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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 28	CA/CAplus patent coverage enhanced
NEWS 3	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 5	JUL 28	STN Viewer performance improved
NEWS 6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 7	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 9	AUG 15	CAplus currency for Korean patents enhanced
NEWS 10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS 12	SEP 25	CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS 14	SEP 29	IFICLS enhanced with new super search field
NEWS 15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS 16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS 17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS 18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS 19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS 20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS 21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

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=> file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
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FILE CONTENT:1840 - 1 Nov 2008 VOL 149 ISS 19

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************************************************************
*                                                          *
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*                                                          *
************************************************************

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Uploading C:\Program Files\Stnexp\Queries\10537723last.str
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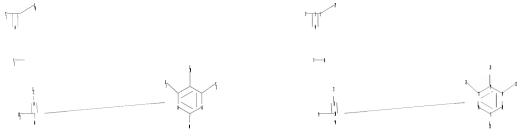


chain nodes :
2 3 4 5 7 8 9 10 11 12 22 23 27 28
ring nodes :
15 16 17 18 19 20
ring/chain nodes :
14 21
chain bonds :
2-3 3-4 3-5 5-27 7-8 9-10 10-11 10-14 11-12 15-21 17-22 18-28 19-23
ring bonds :
15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
2-3 3-4 5-27 7-8 9-10 10-11 10-14 11-12 15-21 17-22 18-28 19-23
exact bonds :
3-5
normalized bonds :
15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
containing 15 :

G1:H,Ak

G2:H,Cb,Ak

G3:C,O,S,N,CN,NO2,Ak

G4:C,H,O,S,N,Cb,Ak,CN,NO2

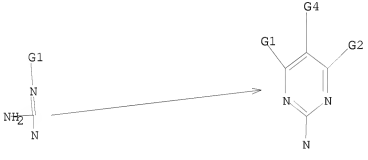
Match level :
2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 23:CLASS 27:CLASS 28:CLASS
fragments assigned product role:

containing 15
fragments assigned reactant/reagent role:
containing 2
containing 7
containing 9

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

G2



G1 H,Ak

G2 H,Cb,Ak

G3 C,O,S,N,CN,NO2,Ak

G4 C,H,O,S,N,Cb,Ak,CN,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 18:21:14 FILE 'CASREACT'
SCREENING COMPLETE - 26134 REACTIONS TO VERIFY FROM 1412 DOCUMENTS

100.0% DONE 26134 VERIFIED 890 HIT RXNS 152 DOCS
SEARCH TIME: 00.00.02

L2 152 SEA SSS FUL L1 (890 REACTIONS)

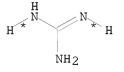
=> s l2 and py<2003
490969 PY<2003

L3 105 L2 AND PY<2003

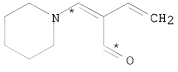
=> d ibib abs fhit tot

L3 ANSWER 1 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 149:266650 CASREACT
TITLE: Guanidine
AUTHOR(S): Palmer, David C.
CORPORATE SOURCE: USA
SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis (2001), No pp. given. John Wiley & Sons, Ltd.: Chichester, UK.
CODEN: 69KUHI
URL: http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME
DOCUMENT TYPE: Conference; General Review; (online computer file)
LANGUAGE: English
AB A review of the article Guanidine.

RX(8) OF 35 ...AC + AA ===> AD

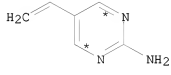


AC



AA

(8)



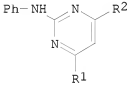
AD

RX(8) RCT AC 113-00-8, AA 85438-16-0
PRO AD 108444-56-0
CAT 124-41-4 NaOMe
SOL 1310-73-2 NaOH
CON 22 deg C
NTE Heterocycle Synthesis: Six-Membered Rings

L3 ANSWER 2 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:423684 CASREACT
TITLE: Preparation of N-(4,6-disubstituted pyrimidin-2-yl)aniline as fungicides
INVENTOR(S): Ma, Yunsheng; Shi, Qingling; Dai, Ronghua
PATENT ASSIGNEE(S): Gao, Mingqiang, Peop. Rep. China; Wang, Zhijiang
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp. CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1385423	A	20021218	CN 2001-118008	20010515

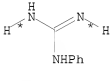
PRIORITY APPLN. INFO.: CN 2001-118008 20010515
OTHER SOURCE(S): MARPAT 140:423684
GI



I

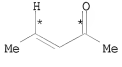
AB Title compds. I (R1 = alkyl, R2 = alkyl, cycloalkyl) are prepared by allowing to react aniline with cyanamide and acid to obtain phenylguanidine salt, then cyclizing with 3-penten-2-one at 30°-150°. Thus, reaction of phenylguanidine sulfate with 3-penten-2-one at 60° for 10 h gave 96.3% 4,6-dimethyl-N-phenyl-2-pyrimidinamine.

RX(1) OF 3 ...A + B ===> C



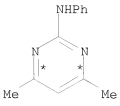
A: CM 1

A: CM 2



B

(1)



C
YIELD 96%

RX(1) RCT A 2498-49-9, B 625-33-2

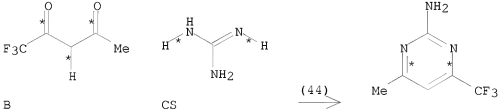
STAGE(1)
CON 10 hours, 60 deg C

STAGE(2)
RGT D 1310-73-2 NaOH
SOL 7732-18-5 Water, 107-06-2 ClCH2CH2Cl

PRO C 53112-28-0

L3 ANSWER 3 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 138:338083 CASREACT
TITLE: Synthesis of fluorinated heterocycles
AUTHOR(S): Sloop, Joseph C.; Bumgardner, Carl L.; Loehle, W. David
CORPORATE SOURCE: Department of Chemistry, United States Military Academy, West Point, NY, 10996, USA
SOURCE: Journal of Fluorine Chemistry (2002), 118(1-2), 135-147
CODEN: JFLCAR; ISSN: 0022-1139
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Selected 1,3-diketones having a trifluoromethyl group and/or a fluorine in the 2-position were condensed with aromatic hydrazines, hydroxylamine, urea, thiourea, guanidine, and substituted anilines producing pyrazoles, isoxazoles, pyrimidines, and quinolines, resp., in yields ranging from 27 to 87%.

RX(44) OF 61 B + CS ===> CT



B CS CT
YIELD 83%

RX(44) RCT B 367-57-7, CS 113-00-8

STAGE(1)
RGT E 7664-93-9 H2SO4
SOL 64-17-5 EtOH
CON 24 - 48 hours, reflux

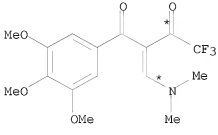
STAGE(2)
RGT F 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON neutralized

PRO CT 5734-63-4
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

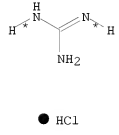
L3 ANSWER 4 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 138:287614 CASREACT
TITLE: Unexpected synthesis of (trifluoroethyl)pyrimidines from the heterocyclization of α-trifluoroacetylpropanenitriles
AUTHOR(S): Berber, Hatice; Soufyane, Mustapha; Santillana-Hayat, Maud; Mirand, Catherine
CORPORATE SOURCE: Universite de Reims Champagne Ardenne, Faculte de Pharmacie, IFR 53, UMR/CNRS 6013, Reims, 51096, Fr.
SOURCE: Tetrahedron Letters (2002), 43(50), 9233-9235
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Some 4-trifluoromethyl-2-aminopyrimidines analogous to trimethoprim and 5-trifluoroethyl-2,4-diaminopyrimidines analogous to pyrimethamine were prepared from enamino(trifluoromethyl)ketones and α-trifluoroacetylpropanenitriles, resp. A novel heterocyclization between a trifluoromethylated β-ketonitrile and guanidine was described.

RX(1) OF 19 A + B ===> C...

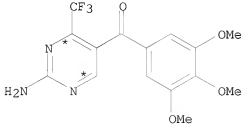


A



B

(1)



C
YIELD 65%

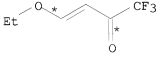
RX(1) RCT A 504408-33-7, B 50-01-1

RGT D 584-08-7 K2CO3
PRO C 504408-35-9
SOL 75-05-8 MeCN
CON 65 deg C
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

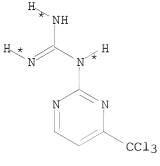
L3 ANSWER 5 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 138:238114 CASREACT
TITLE: Synthesis of 4-(trihalomethyl)dipyrimidin-2-ylamines from β-alkoxy-α,β-unsaturated trihalomethyl ketones
AUTHOR(S): Zanatta, Nilo; Lopes, Elizandra C. S.; Fantinel, Leonardo; Bonacorso, Helio G.; Martins, Marcos A. P.
CORPORATE SOURCE: Nucleo de Quimica de Heterociclos (NUQUIMHE), DEp. de Quimica, Univ. Federal de Santa Maria, Santa Maria, Brazil
SOURCE: Journal of Heterocyclic Chemistry (2002), 39(5), 943-947
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of a novel series of twelve (2-pyrimidinyl)[4-(trihalomethyl)-2-pyrimidinyl]amines, from the cyclocondensation reaction of [4-(trichloromethyl)-2-pyrimidinyl]guanidine with β-alkoxyvinyl trihalomethyl ketones was reported. The reactions were carried out in acetonitrile under reflux for 16 h, leading to the bis[4-(halomethyl)-2-pyrimidinyl]amines in 65-90% yield. Depending on the substituents of the vinyl ketone, tetrahydropyrimidines or aromatic pyrimidine rings were obtained from the cyclization reaction. For 1,1,1-trichloro-4-alkoxy-2-alken-2-one derivs., elimination of the trichloromethyl group was observed during the cyclization step. The structure of [4-(trihalomethyl)-2-pyrimidinyl]amines was studied in detail by 1H-, 13C- and 2D-NMR spectroscopy.

RX(1) OF 10 A + B ===> C

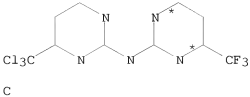


A



B

(1)

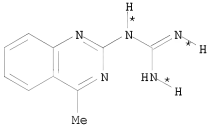


C
YIELD 87%

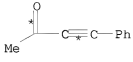
```
RX(1)      RCT  A 17129-06-5, B 380305-28-2
           PRO  C 502162-64-3
           SOL  75-05-8 MeCN
           CON  16 hours, reflux
REFERENCE COUNT:         37     THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

L3 ANSWER 6 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 137:352985 CASREACT
TITLE: 2-Quinazolylguanidines in heterocyclization reactions. Part 2. Condensation with α,β-unsaturated carbonyl compounds
AUTHOR(S): Shikhaliev, Kh. S.; Falaleev, A. V.; Ermolova, G. I.; Solov'ev, A. S.
CORPORATE SOURCE: Voronezh State University, Voronezh, 394693, Russia
SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2002), 38(2), 210-212
CODEN: CHCCAL; ISSN: 0009-3122
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 4,4,6-Trimethyl-1,4-dihydropyrimidines were synthesized by condensation of 2-quinazolylguanidines with mesityl oxide. The analogous reaction with benzal-acetone leads to unstable 6-methyl-4-phenyl-1,4-dihydropyrimidines, which are oxidized to the corresponding 4-methyl-6-phenylpyrimidines.

RX(1) OF 9 A + B ===> C



A



B

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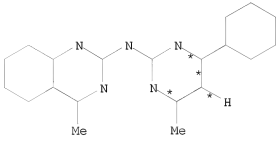


C
YIELD 47%

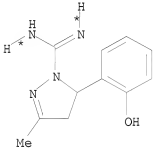
RX(1) RCT A 716-11-0, B 1817-57-8

PRO C 351225-60-0
SOL 67-68-5 DMSO
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

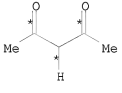
L3 ANSWER 7 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 137:352947 CASREACT
TITLE: Novel heterocycles containing the pyrazole unit
AUTHOR(S): Svetlik, Jan; Liptaj, Tibor
CORPORATE SOURCE: Department of Pharmaceutical Analysis and Nuclear Pharmacy, Faculty of Pharmacy, Comenius University, Bratislava, SK-832 32, Slovakia
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (10), 1260-1265
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New condensed pyrazolo[1,5-e][1,3,5]benzoxadiazocine and bridged 5,11-methano-[1,2,4]triazolo[1,2-c][1,3,4]benzoxadiazepine heterocyclic ring systems were prepared by cyclizations of 4,5-dihydro-3-methyl-5-(2-hydroxyphenyl)-1H-pyrazole-1-carboximidamide with C1 reagents (tri-Et orthoformate and 1,1'-carbonyldiimidazole). In contrast, cyclocondensations with C2 and C3 reactants occur exclusively at the amidine moiety yielding substituted pyrano[2,3-d]pyrimidine, pyrimidine, and imidazole derivs.

RX(10) OF 12 A + V ===> W

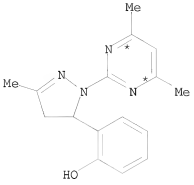


A



V

(10)



W
YIELD 73%

RX(10) RCT A 460060-12-2, V 123-54-6
PRO W 474938-37-9
SOL 68-12-2 DMF
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 105 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 137:279157 CASREACT

TITLE: Synthesis and biological activity of N-(substituted benzoyl)-N'-(1,2,4-triazolo[1,5-α]pyrimidinyl) thioureas

AUTHOR(S): Wang, Sheng; Liu, Dan; Feng, Gui-Rong; Gong, Yin-Xiang; Wang, Yan-Gang

CORPORATE SOURCE: Department of Chemistry, Central China Normal University, Wuhan, 430079, Peop. Rep. China

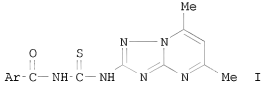
SOURCE: Huazhong Shifan Daxue Xuebao Zirankexueban (2001), 35(2), 176-179
CODEN: HDZKEL; ISSN: 1000-1190

PUBLISHER: Huazhong Shifan Daxue Xuebao Bianjibu

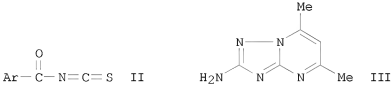
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



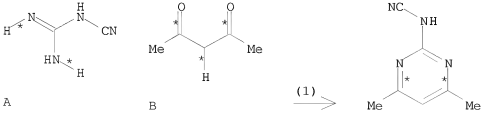
I



II III

AB Title compds. I (Ar = p-chlorophenyl, p-bromophenyl, p-nitrophenyl, o-chlorophenyl, m-chlorophenyl, m-nitrophenyl, m,o-dinitrophenyl)were synthesized via condensation of II and III, and characterized by the methods of UV, IR, 1HNMR and elementary anal.. Primary expts. indicated that target compds. have better herbicidal activity in consistency of 100 mg/L, and have good plant regulating activity in consistency of 10 mg/L.

RX(1) OF 34 A + B ===> C...



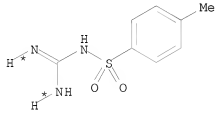
A B (1) C

YIELD 60%

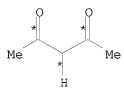
RX(1) RCT A 461-58-5, B 123-54-6
       RGT D 1310-73-2 NaOH
       PRO C 55474-90-3
       SOL 7732-18-5 Water

L3 ANSWER 9 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 137:169483 CASREACT
TITLE: (Arylsulfonyl)guanidines in synthesis of pyrimidinyl sulfonamides. I
AUTHOR(S): Farzaliev, V. M.; Shakhgel'dieva, L. M.; Mamedov, S. A.; Ladokhina, N. P.
CORPORATE SOURCE: Inst. Khim. Prisadok im. A. M. Kulieva, AN Azerbaidzhana, Azerbaijan
SOURCE: Azerbaidzhanskii Khimicheskii Zhurnal (2001), (1), 7-9
CODEN: AZKZAU; ISSN: 0005-2531
PUBLISHER: Natsional'naya Akademiya Nauk Azerbaidzhana
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Preparation of pyrimidines by reactions of (arylsulfonyl)guanidines with unsatd. ketones and 1,3-diketones are studied.

RX(3) OF 18 ...C + I ===> J

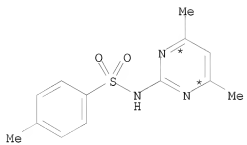


C



I

(3)



J
YIELD 87%

RX(3) RCT C 6584-12-9, I 123-54-6

STAGE(1)
SOL 64-17-5 EtOH

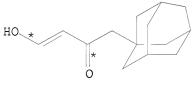
STAGE(2)
RGT D 1310-73-2 NaOH

SOL 64-17-5 EtOH

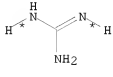
PRO J 123458-65-1

L3 ANSWER 10 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 136:355209 CASREACT
TITLE: Syntheses of heterocycles from the sodium salts of 3-(1-adamantyl)-1-hydroxy-1-propen-3-one and 4-(1-adamantyl)-1-hydroxy-1-buten-3-one
AUTHOR(S): Makarova, N. V.; Zemtsova, M. N.; Moiseev, I. K.
CORPORATE SOURCE: Samara State Technical University, Samara, 443100, Russia
SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2001), 37(7), 840-843
CODEN: CHCCAL; ISSN: 0009-3122
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interaction of the Na salts of 3-(1-adamantyl)-1-hydroxy-1-propen-3-one and 4-(1-adamantyl)-1-hydroxy-1-buten-3-one with hydroxylamine, hydrazine, and guanidine gives 5-(1-adamantyl)-5-hydroxy- and 5-(1-adamantylmethyl)-5-hydroxy-Δ2-isoxazolines, 3-(1-adamantyl)- and 3-(1-adamantylmethyl)pyrazoles, 3-(1-adamantyl)-2-phenylpyrazole, and 4-(1-adamantyl)-2-amino- and 4-(1-adamantylmethyl)-2-aminopyrimidines.

RX(7) OF 10 F + M ===> O



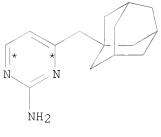
F



M: CM 1

M: CM 2

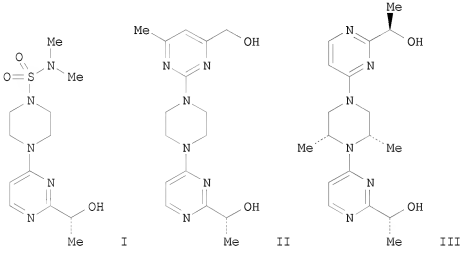
(7)



O
YIELD 70%

RX(7) RCT F 420088-18-2, M 506-93-4
PRO O 420088-17-1
SOL 64-17-5 EtOH, 7732-18-5 Water
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 136:200160 CASREACT
TITLE: Orally-Effective, Long-Acting Sorbitol Dehydrogenase Inhibitors: Synthesis, Structure-Activity Relationships, and in Vivo Evaluations of Novel Heterocycle-Substituted Piperazino-Pyrimidines
AUTHOR(S): Chu-Moyer, Margaret Y.; Ballinger, William E.; Beebe, David A.; Berger, Richard; Coutcher, James B.; Day, Wesley W.; Li, Jiancheng; Mylari, Banavara L.; Oates, Peter J.; Weekly, R. Matthew
CORPORATE SOURCE: Groton Laboratories, Departments of Cardiovascular and Metabolic Disease and Drug Metabolism Development, Pfizer Global Research and Development, Groton, CT, 06340, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(2), 511-528
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



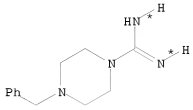
I II III

AB Optimization of a previously disclosed sorbitol dehydrogenase inhibitor (SDI, I) for potency and duration of action was achieved by replacing the metabolically labile N,N-dimethylsulfamoyl group with a variety of heterocycles. Specifically, this effort led to a series of novel, in vitro potent SDI's, e.g. the [[(hydroxymethylpyrimidinyl)piperazinyl]pyrimidinyl]ethanol II, with longer serum half-lives and acceptable in vivo activity in acutely diabetic rats. However, the desired in vivo potency in chronically diabetic rats, ED90 ≤ 5 mg/kg/day, was achieved only through further modification of the piperazine linker. Several members of this family, including [[(hydroxyethylpyrimidinyl)dimethylpiperazinyl]pyrimidin yl]ethanol III, showed better than the targeted potency with ED90 values of 1-2 mg/kg/day. III was further profiled and found to be a selective inhibitor of sorbitol dehydrogenase, with excellent

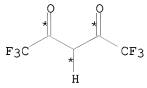
pharmacodynamic/pharmacokinetic properties, demonstrating normalization of sciatic nerve fructose in a chronically diabetic rat model for .apprx.17 h, when administered orally at a single dose of 2 mg/kg/day.

RX(45) OF 265 CI + CJ ===> CK...

CI: CM 1

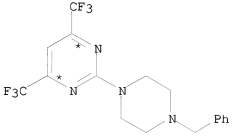


CI: CM 2



CJ

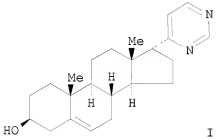
(45)



CK
YIELD 100%

RX(45) RCT CI 400785-35-5, CJ 1522-22-1
RGT CL 683-60-3 NaOPr-i
PRO CK 400785-31-1
SOL 67-63-0 Me2CHOH
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

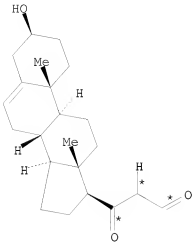
L3 ANSWER 12 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 136:102563 CASREACT
TITLE: Syntheses and pharmacological activity of some 17-[(2'-substituted)-4'-pyrimidyl]androstene derivatives as inhibitors of human 17α-hydroxylase/C17,20-lyase
AUTHOR(S): Ru, Chengjie; Lei, Xiaoping; Ling, Yangzhi; Zhang, Lihe; Hundratta, Venkatech; Brodie, Angela
CORPORATE SOURCE: School of Pharmaceutical Sciences, Peking University, Beijing, 100083, Peop. Rep. China
SOURCE: Journal of Chinese Pharmaceutical Sciences (2001), 10(1), 3-8
CODEN: JCHSE4; ISSN: 1003-1057
PUBLISHER: Beijing Medical University, School of Pharmaceutical Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



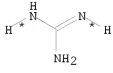
I

AB 17-Heterocyclic substituted androstene derivs. have been found to be potent inhibitors for human testicular microsomal 17α-hydroxylase/C17,20-lyase, which have potential usage in the treatment of benign prostatic hypertrophy(BPH) and prostatic cancer. In order to further investigate their structure-activity relationships, seven new 17-[(2'-substituted)-4'-pyrimidyl]androstene derivs. were designed and synthesized. The structures of the compds. were confirmed by IR, 1H NMR, elemental anal. or MS measurements. The results of the pharmacol. activity tests showed that compound I is a potent inhibitor for P 45017α with IC50 225 nmol·L-1.

RX(2) OF 5 A + F ===> G



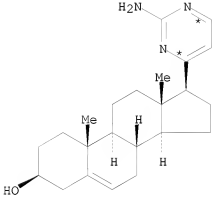
A



F: CM 1

F: CM 2

(2)



G
YIELD 25%

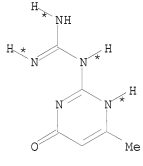
RX(2) RCT A 10163-90-3, F 100224-74-6
PRO G 388083-12-3
SOL 7732-18-5 Water, 64-17-5 EtOH
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 105 CASREACT COPYRIGHT 2008 ACS on STN

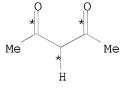
ACCESSION NUMBER: 136:85589 CASREACT
TITLE: A Multiple Hydrogen-Bond Scaffold Based on Dipyrimidin-2-ylamine
AUTHOR(S): Soentjens, Serge H. M.; Meijer, Joris T.; Kooijman, Huub; Spek, Anthony L.; van Genderen, Marcel H. P.; Sijbesma, Rint P.; Meijer, E. W.
CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Organic Letters (2001), 3(24), 3887-3889
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A multiple hydrogen-bond array based on dipyrimidin-2-ylamine is presented, which is easily accessible. The influence of a preorganizing intramol. hydrogen bond, tautomeric equilibrium, and steric effects on the association behavior were investigated. X-ray diffraction shows that the mols. feature an ADA (acceptor-donor-acceptor) array of hydrogen-bonding sites in the solid state. The array persists in solution, and 1H NMR titrns. show that mols. with sterically nondemanding DAD arrays are selectively bound.

RX(4) OF 20 ...J + M ===> N

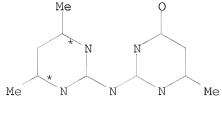


J



M

(4)



N

YIELD 50%

RX(4) RCT J 78224-73-4, M 123-54-6

STAGE(1)
RGT O 64-19-7 AcOH
SOL 7732-18-5 Water

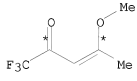
STAGE(2)
RGT P 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO N 387821-55-8
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

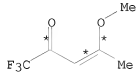
L3 ANSWER 14 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 135:318474 CASREACT
TITLE: Regiospecific cyclization of β-methoxyvinyl trifluoromethyl ketones with aminoguanidine: a convenient method to obtain trifluoromethylated 2-[1H-pyrazol-1-yl]pyrimidines
AUTHOR(S): Bonacorso, Helio Gauze; Wentz, Alexandre Pereira; Zanatta, Nilo; Martins, Marcos Antonio Pinto
CORPORATE SOURCE: Nucleo de Quimica de Heterociclos (NUQUIMHE), Departamento de Quimica, Universidade Federal de Santa Maria, Santa Maria, 97105-900, Brazil
SOURCE: Synthesis (2001), (10), 1505-1508
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The regiospecific one-pot synthesis of a novel series of 6-alkyl(aryl)-2-[3-alkyl(aryl)-5-trifluoromethyl-5-hydroxy-4,5-dihydro-1H-pyrazol-1-yl]-4-trifluoromethylpyrimidines and 6-alkyl(aryl)-2-[3-alkyl(aryl)-5-trifluoromethyl-1H-pyrazol-1-yl]-4-trifluoromethylpyrimidines from 4-alkyl(aryl)-1,1,1-trifluoro-4-methoxyalk-3-en-2-ones and aminoguanidine bicarbonate is reported.

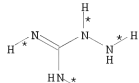
RX(1) OF 12 2 A + B ===> C...



A



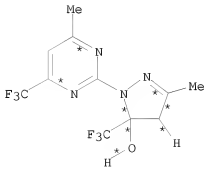
A



B: CM 1

B: CM 2

(1)



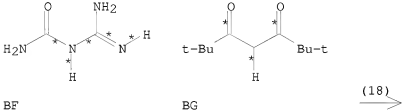
C
YIELD 85%

RX(1) RCT A 102145-82-4, B 2582-30-1
PRO C 368422-53-1
SOL 67-56-1 MeOH
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

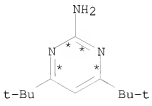
L3 ANSWER 15 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 134:29571 CASREACT
TITLE: Retinoidal pyrimidinecarboxylic acids. Unexpected diaza-substituent effects in retinobenzoic acids
AUTHOR(S): Ohta, Kiminori; Kawachi, Emiko; Inoue, Noriko; Fukasawa, Hiroshi; Hashimoto, Yuichi; Itai, Akiko; Kagechika, Hiroyuki
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, 113-0033, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2000), 48(10), 1504-1513
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several pyridine- and pyrimidine-carboxylic acids were synthesized as ligand candidates for retinoid nuclear receptors, retinoic acid receptors (RARs) and retinoic X receptors (RXRs). Although the pyridine derivs., 6-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)carbamoyl]pyridine-3-carboxylic acid and 6-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)carboxamido]pyridine-3-carboxylic acid are more potent than the corresponding benzoic acid-type retinoids, Am80 and Am580, the replacement of the benzene ring of Am580, Am555, or Am55 with a pyrimidine ring caused loss of the retinoidal activity both in HL-60 cell differentiation assay and in RAR transactivation assay using COS-1 cells. On the other hand, pyrimidine analogs (PA series) of potent RXR agonists (retinoid synergists) with a diphenylamine skeleton (DA series) exhibited potent retinoid synergistic activity in HL-60 cell differentiation assay and activated RXRs. Among the synthesized compds., 2-[N-n-propyl-N-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)amino]pyrimidine-5-carboxylic acid (PA013) is most active retinoid synergist in HL-60 assay.

RX(18) OF 115 ...BF + BG ===> BH...



BF BG



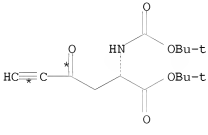
BH
YIELD 62%

RX(18) RCT BF 141-83-3, BG 1118-71-4
PRO BH 78641-13-1
SOL 7732-18-5 Water, 64-17-5 EtOH
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

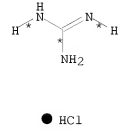
L3 ANSWER 16 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 131:73920 CASREACT
TITLE: The synthesis of pyrimidin-4-yl substituted α-amino acids. A versatile approach from alkynyl ketones
AUTHOR(S): Adlington, Robert M.; Baldwin, Jack E.; Catterick, David; Pritchard, Gareth J.
CORPORATE SOURCE: The Dyson Perrins Laboratory, University of Oxford, Oxford, OX1 3QY, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (8), 855-866
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reaction of amidines with α-amino acid alkynyl ketones is shown to be a versatile route to pyrimidin-4-yl substituted α-amino acids. This route is also applicable to a parallel synthesis approach and has allowed the formation of a range of pyrimidin-4-yl substituted α-amino acids, including the naturally occurring α-amino acid L-lathyrine.

RX(15) OF 21 COMPOSED OF RX(3), RX(4), RX(5)
RX(15) L + P + Q ===> X



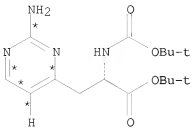
L



P

Q

3
STEPS



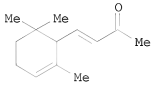
X
YIELD 93%

RX(3) RCT L 197159-35-6, P 50-01-1, Q 75-08-1
RGT S 497-19-8 Na2CO3
PRO R 197159-61-8
SOL 141-78-6 AcOEt, 7732-18-5 Water

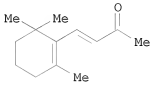
RX(4) RCT R 197159-61-8
RGT V 937-14-4 MCPBA
PRO U 197159-73-2
SOL 75-09-2 CH2Cl2

RX(5) RCT U 197159-73-2
RGT Y 7664-41-7 NH3
PRO X 197159-82-3
SOL 109-99-9 THF
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

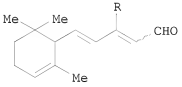
L3 ANSWER 17 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 130:209663 CASREACT
TITLE: Synthesis of new heterocyclic derivatives of retinoids
AUTHOR(S): Sottofattori, Enzo; Anzaldi, Maria; Balbi, Alessandro
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Genoa, 3, Italy
SOURCE: Journal of Heterocyclic Chemistry (1998), 35(6), 1377-1380
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II



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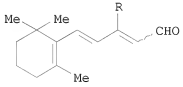
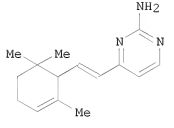


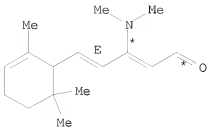
IV



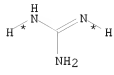
V

AB Reaction of α- and β-ionones I and II with dialkylformamide/phosphorus oxychloride affords enamines III (R = Me2N, Et2N) and IV (R = Me2N) along with the expected chloro derivs. III and IV (R = Cl). Reaction of III (R = Me2N) with hydrazines, hydroxylamine and guanidine furnished pyrazole, isoxazole, pyrimidine derivs., e.g. V, showing the potential of these enaminones as key intermediates in the synthesis of synthetic retinoids.

RX(5) OF 9 ...D + P ===> Q



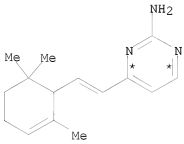
D



P: CM 1

P: CM 2

(5)



Q
YIELD 85%

RX(5) RCT D 220968-18-3, P 100224-74-6
PRO Q 220968-24-1
SOL 64-17-5 EtOH, 7732-18-5 Water
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 125:212675 CASREACT
TITLE: 1,4,5-Trisubstituted imidazoles useful as cytokine suppressors
INVENTOR(S): Adams, Jerry Leroy; Gallagher, Timothy F.; Garigipati, Ravi Shanker; Boehm, Jeffrey Charles; Sisko, Joseph; Peng, Zhi-Qiang; Lee, John Cheung-Lun
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9621452	A1	19960718	WO 1996-US546	19960111
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5593992	A	19970114	US 1995-472366	19950607
ZA 9600094	A	19960724	ZA 1996-94	19960108
AU 9646572	A	19960731	AU 1996-46572	19960111
AU 705207	B2	19990520		
BR 9606904	A	19971021	BR 1996-6904	19960111
EP 809499	A1	19971203	EP 1996-902151	19960111
EP 809499	B1	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI				
JP 10512555	T	19981202	JP 1996-521862	19960111
JP 3330952	B2	20021007		
RU 2196139	C2	20030110	RU 1997-113753	19960111
AT 254613	T	20031215	AT 1996-902151	19960111
BG 63769	B1	20021229	BG 1997-101727	19970702
FI 9702901	A	19970908	FI 1997-2901	19970708
NO 9703167	A	19970908	NO 1997-3167	19970708
HK 1003623	A1	20041029	HK 1998-103016	19980409
NO 2001006225	A	19970908	NO 2001-6225	20011219
NO 2001006226	A	19970908	NO 2001-6226	20011219

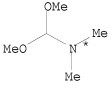
PRIORITY APPLN. INFO.: US 1995-369964 19950109
US 1995-472366 19950607
US 1993-92733 19930716
WO 1996-US546 19960111

OTHER SOURCE(S): MARPAT 125:212675
GI

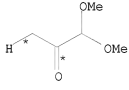
I

AB Imidazole derivs. I [R1 = (substituted) 4-pyridyl, pyrimidinyl, quinolyl, isoquinolyl, quinazolin-4-yl, 1-imidazolyl, 1-benzimidazolyl; R2 = (substituted) C1-10 alkyl, C2-10 alkenyl or alkynyl, N3, cycloalkyl, heterocyclyl, etc.; R4 = (substituted) Ph, 1- or 2-naphthyl, heteroaryl] are prepared which inhibit mitogen-activated protein kinase and the secretion of interleukin 1 and tumor necrosis factor and are useful in treatment of cytokine-mediated inflammatory diseases. Thus, 1-[3-(4-morpholinyl)propyl]-4-(4-fluorophenyl)-5-(4-pyridyl)imidazole (II) inhibited lipopolysaccharide-induced prostaglandin endoperoxide synthase-2 expression in human monocytes with a potency similar to that of dexamethasone. II was prepared by condensation of pyridine-4-carboxaldehyde with 4-(3-aminopropyl)morpholine and reaction of the product with 4-fluorophenyl-tolylthiomethylisocyanide (prepared from p-fluorobenzaldehyde, thiocresol, and HCONH2).

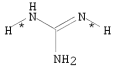
RX(30) OF 191 BZ + CA + CB ===>
X...



BZ



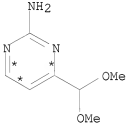
CA



● HCl

CB

(30)



X
YIELD 50%

RX(30) RCT BZ 4637-24-5, CA 6342-56-9

STAGE(1)

STAGE(2)
RCT CB 50-01-1

RGT AT 1310-73-2 NaOH
SOL 7732-18-5 Water

PRO X 165807-05-6
NTE THERMAL FIRST STAGE

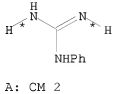
L3 ANSWER 19 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 125:114684 CASREACT
TITLE: Process for the preparation of 2-anilino-pyrimidine derivatives
INVENTOR(S): Ressel, Hans-Joachim; Schlegel, Guenter
PATENT ASSIGNEE(S): Hoechst Schering AgrEvo GmbH, Germany
SOURCE: Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 717038	A1	19960619	EP 1995-113519	19950829
EP 717038	B1	19981118		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
DE 4444928	A1	19960627	DE 1994-4444928	19941216
AT 173472	T	19981215	AT 1995-113519	19950829
ES 2124942	T3	19990216	ES 1995-113519	19950829

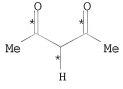
PRIORITY APPLN. INFO.: DE 1994-4444928 19941216
OTHER SOURCE(S): MARPAT 125:114684
AB 2-Anilinopyrimidines were prepared by the reaction of phenylguanidinium salts with β-diketones.

RX(1) OF 1 A + B ===> C

A: CM 1

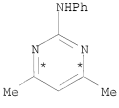


A: CM 2



B

(1)



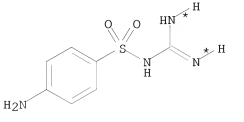
C
YIELD 99%

RX(1) RCT A 6685-76-3, B 123-54-6
PRO C 53112-28-0

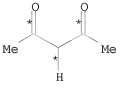
L3 ANSWER 20 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 123:339989 CASREACT
TITLE: Condensation between sulfaguanidine and acetylacetone for synthesizing sulfadimidine
AUTHOR(S): Mai, Tuyen; Ngo Dai Quang; Tran Minh Yen
CORPORATE SOURCE: Inst. of Chemistry, Vietnam
SOURCE: Tap Chi Hoa Hoc (1994), 32(3), 32-4
CODEN: TCHHDC; ISSN: 0378-2336
PUBLISHER: Toa Soan Tap Chi Hoa Hoc
DOCUMENT TYPE: Journal
LANGUAGE: Vietnamese

AB The condensation between sulfaguanidine and acetylacetone was studied in various media, such as water, ethanol or acetic acid. The exptl. results obtained showed that the acidity of the reaction mixture exerts certain influence on the reaction velocity. In order to elucidate this factor the condensation reaction was investigated with a variety of pH values. The exptl. data demonstrated that the desired product could be prepared in higher yield if the weak acidity of the reaction mixture was maintained by using a buffer solution

RX(1) OF 4 A + B ===> C

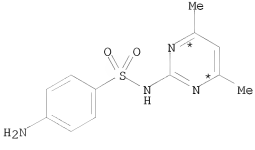


A



B

(1)



C
YIELD 78%

RX(1) RCT A 57-67-0, B 123-54-6
PRO C 57-68-1
NTE 30 H, 140.deg.

L3 ANSWER 21 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 123:55916 CASREACT
TITLE: Preparation of crystal modification B of (4-cyclopropyl-6-methyl-pyrimidin-2-yl)phenylamine as a fungicide.
INVENTOR(S): Baettig, Willy; Hanreich, Reinhard Georg
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

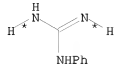
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 655441	A1	19950531	EP 1994-810626	19941101
EP 655441	B1	20020123		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 212337	T	20020215	AT 1994-810626	19941101
PT 655441	T	20020628	PT 1994-810626	19941101
ES 2171443	T3	20020916	ES 1994-810626	19941101
CA 2135251	A1	19950510	CA 1994-2135251	19941107
CA 2135251	C	20051220		
FI 9405231	A	19950510	FI 1994-5231	19941107
FI 112215	B1	20031114		
PL 179802	B1	20001031	PL 1994-305740	19941107
IL 111537	A	20010614	IL 1994-111537	19941107
SK 282969	B6	20030109	SK 1994-1330	19941107
CZ 291977	B6	20030618	CZ 1994-2730	19941107
ZA 9408815	A	19950509	ZA 1994-8815	19941108
NO 9404253	A	19950510	NO 1994-4253	19941108
AU 9477688	A	19950518	AU 1994-77688	19941108
AU 689805	B2	19980409		
BR 9404388	A	19950704	BR 1994-4388	19941108
HU 68779	A2	19950728	HU 1994-3214	19941108
HU 213946	B	19971128		
JP 07188183	A	19950725	JP 1994-300401	19941109
JP 3617015	B2	20050202		
CN 1105995	A	19950802	CN 1994-118186	19941109
CN 1053897	C	20000628		
RU 2145601	C1	20000220	RU 1994-40724	19941109
US 5830899	A	19981103	US 1997-909491	19970812
HK 1008961	A1	20021220	HK 1998-109715	19980805
PRIORITY APPLN. INFO.:			CH 1993-3368	19931109
			CH 1994-2393	19940728
			US 1994-330274	19941027
			US 1996-692303	19960805

AB Title compound (I) having ≥98% eutectic purity, a melting pt. of >73°, preferably 73-75°, and specified IR bands and X-ray powder diffraction pattern, was prepared Thus, phenylguanidine carbonate and 1-cyclopropyl-1,3-butanedione were heated in methylcyclohexane with azeotropic distillation of H2O; solvent was removed using, e.g., a falling film apparatus and the product at 74° was introduced into a vessel equipped with a rotating arm for removing I crystals from the walls of the vessel (walls maintained at 50°). I had superior storage stability relative to crystal modification A; I as a 0.006% spray gave 90-100%

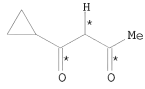
control of Venturia inaequalis on apple cuttings.

RX(1) OF 1 A + B ===> C

A: CM 1

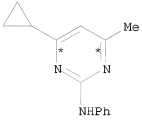


A: CM 2



B

(1)



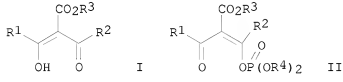
C

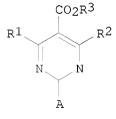
RX(1) RCT A 6291-89-0, B 21573-10-4
PRO C 121552-61-2
SOL 108-87-2 Methylcyclohexane
NTE THIS PATENT IS MOSTLY ABOUT OBTAINING A SPECIFIC CRYSTALLINE FORM OF THE PRODUCT

L3 ANSWER 22 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 122:56049 CASREACT
TITLE: Method for synthesis of 5-alkoxycarbonylpyrimidine derivatives
INVENTOR(S): Koike, Haruo; Kabaki, Mikio; Watanabe, Masamichi
PATENT ASSIGNEE(S): Shionogi Seiyaku Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06256318	A	19940913	JP 1993-40248	19930301
JP 3197971	B2	20010813		

PRIORITY APPLN. INFO.: JP 1993-40248 19930301
OTHER SOURCE(S): MARPAT 122:56049
GI

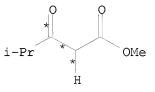




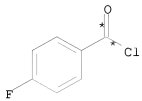
AB Diketone carboxylic acid enol [I; R1 - R3 = H, each (un)substituted alkyl, aralkyl, aryl, or heteroaryl] is reacted with (R4O)2P(O)X1 [R4 = each (un)substituted alkyl, aralkyl, aryl, or heteroaryl; X1 = halo] in the presence of a base to give enol phosphate ester (II; R1 -R4 = same as above) which is cyclocondensed with amidine A-C(:NH)NH2 [A = alkyl, aralkyl, aryl, SR5, OR6, NR6R7; R5 - R8 = H, each (un)substituted alkyl, aryl, heteroaryl, aralkyl, alkylsulfonyl, or arylsulfonyl] in the presence of a base to give the title 5-alkoxycarbonylpyrimidine derivs. (III; R1 -R3, A = same as above). This process efficiently gives III in an industrial scale which is useful as an intermediate for 3-hydroxy-3-methylglutaryl-CoA (HMG-CoA) inhibitor. Thus, 7.72 g 10% aqueous NaOH was added dropwise over 10 min to a solution of 4.32 g Me isobutyrylacetate in toluene under ice-cooling followed by adding dropwise 7.27 g 33% aqueous NaOH and 5.13 g p-fluorobenzoyl chloride over 43 min and the resulting mixture was gradually warmed to room temperature with stirring for 1 h to give 85.6% I (R1 = 4-fluorophenyl, R2 = iso-Pr, R3 = Me). The latter compound (7.99 g) was dissolved 80 mL MeCN followed by adding 2.34 g Et3N

under ice-cooling followed by stirring for 10 min and adding 8.87 g di-Ph chlorophosphate and the resulting mixture was stirred for 4 h to give 64.2% II (R1 = 4-fluorophenyl, R2 = iso-Pr, R3 = Me, R4 = Ph). To the latter phosphate ester (1.99 g) was added a mixture of 0.72 g S-methylisothiourea sulfate, 0.64 g K2CO3, and 10 mL DMSO and the resulting mixture was stirred at 90° for 7 h to give 21% pyrimidine derivative III (R1 = 4-fluorophenyl, R2 = iso-Pr, R3 = Me, A = SMe).

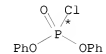
RX(11) OF 12 COMPOSED OF RX(1), RX(2), RX(4)
RX(11) A + B + G + O ===> P



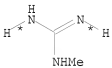
A



B



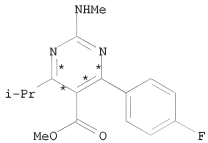
G



O

● HCl

3
STEPS



P
YIELD 42%

RX(1) RCT A 42558-54-3, B 403-43-0
RGT D 1310-73-2 NaOH
PRO C 160009-32-5
SOL 7732-18-5 Water, 108-88-3 PhMe
NTE ice-cooling to room temp.

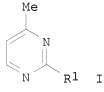
RX(2) RCT C 160009-32-5, G 2524-64-3
RGT I 121-44-8 Et3N
PRO H 160009-34-7
SOL 75-05-8 MeCN
NTE ice-cooling

RX(4) RCT H 160009-34-7, O 21770-81-0
RGT Q 124-41-4 NaOMe
PRO P 160009-36-9
SOL 67-56-1 MeOH
NTE reflux for 1.5 h

L3 ANSWER 23 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 121:255823 CASREACT
TITLE: Preparation of 4-methylpyrimidines
INVENTOR(S): Rittinger, Stefan; Rieber, Norbert
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 6 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4308073	A1	19940915	DE 1993-4308073	19930313
US 5414086	A	19950509	US 1994-199452	19940222
EP 620217	A1	19941019	EP 1994-103290	19940304
EP 620217	B1	19960529		

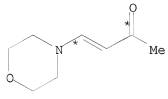
R: BE, CH, DE, FR, GB, IT, LI, NL
PRIORITY APPLN. INFO.: DE 1993-4308073 19930313
OTHER SOURCE(S): MARPAT 121:255823
GI



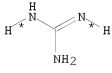
I

AB Title compds. [I; R1 = (cyclo)alkyl, aryl, OH, NH2, etc.] were prepared by cyclocondensation of R2R3NCH:CHCOMe (II; R2,R3 = alkyl, aryl, etc.; R2R3 = atoms to form a ring) with R1C(:X)NH2. Thus, II (NR2R3 = morpholino)(preparation from morpholine and HC.tplbond.CC.tplbond.CH given) was cyclocondensed with guanidine to give I (R1 = NH2).

RX(2) OF 5 ...C + E ===> F



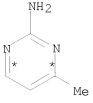
C



E: CM 1

E: CM 2

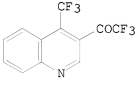
(2)



F
YIELD 75%

RX(2) RCT C 6051-55-4, E 593-85-1
PRO F 108-52-1
SOL 1330-20-7 Xylene

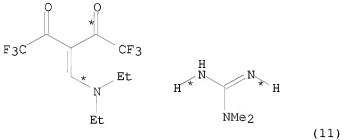
L3 ANSWER 24 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 121:9306 CASREACT
TITLE: Synthesis of some fluorinated nitrogen heterocycles from (diethylaminomethylene)hexafluoroacetylacetone (DAMFA)
AUTHOR(S): Soufyane, Mustapha; Mirand, Catherine; Levy, Jean
CORPORATE SOURCE: Fac. Pharm., Univ. Reims Champagne-Ardenne, Reims, F 51096, Fr.
SOURCE: Tetrahedron Letters (1993), 34(48), 7737-40
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



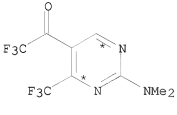
I

AB Simple and highly efficient syntheses of the title compds. from DAMFA are described in the quinoline, e.g., I, azepinonaphthalene, azaphenanthrene, pyridopyridine, pyrazole, pyrrole and pyrimidine series.

RX(11) OF 17 K + W ===> X



K W (11)

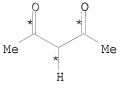


X
YIELD 85%

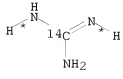
RX(11) RCT K 74888-65-6, W 6145-42-2
        PRO X 155495-80-0
        SOL 75-05-8 MeCN

L3 ANSWER 25 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 120:279550 CASREACT
TITLE: Comparative characteristics of the stability of sulfonyl urea herbicides in bodies of water
AUTHOR(S): Khalikov, I. S.; Pomeshchikov, V. D.; Savin, Yu. I.
CORPORATE SOURCE: USSR
SOURCE: Tr. In-ta Ekserim. Meteorol. Goskomgidromet (1991), (20), 10-21
From: Ref. Zh., Khim. 1992, Abstr. No. 10O443
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.

RX(2) OF 6 C + D ===> E...

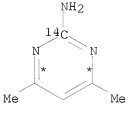


C



D

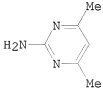
(2)



E
YIELD 64%

RX(2) RCT C 123-54-6, D 87862-39-3
PRO E 124475-81-6

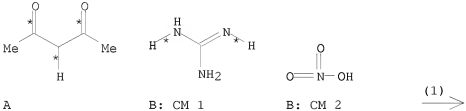
L3 ANSWER 26 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 120:77254 CASREACT
TITLE: Synthesis of 2-amino-4,6-dimethylpyrimidine
AUTHOR(S): Xue, Sijia; Zhang, Aidong; Wang, Haitao
CORPORATE SOURCE: Dep. Chem., Cent. China Norm. Univ., Wuhan, 430070, Peop. Rep. China
SOURCE: Huaxue Shiji (1993), 15(3), 181
CODEN: HUSHDR; ISSN: 0258-3283
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



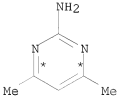
I

AB Treating guanidine nitrate with acetylacetone and K2CO3 in H2O at room temperature for 24 h gave 97% the title compound (I).

RX(1) OF 1 A + B ===> C



A B: CM 1 B: CM 2 (1)

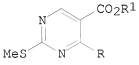


C
YIELD 97%

RX(1) RCT A 123-54-6, B 506-93-4
RGT D 584-08-7 K2CO3

PRO C 767-15-7
SOL 7732-18-5 Water

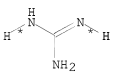
L3 ANSWER 27 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 119:151683 CASREACT
TITLE: Reaction of 2-dimethylaminomethylene-1,3-diones with dinucleophiles. Part XI. Synthesis, antiviral (HSV-1) and antimycotic activities of ethyl or methyl 2,4-disubstituted 5-pyrimidinecarboxylates, 2,4-disubstituted 5-pyrimidinecarboxylic acids and 2,4-disubstituted pyrimidines
AUTHOR(S): Sansebastiano, Laura; Mosti, Luisa; Menozzi, Giulia; Schenone, Pietro; Muratore, Olimpio; Petta, Andrea; Debbia, Eugenio; Schito, Adelaide Pesce; Schito, Gian Carlo
CORPORATE SOURCE: Ist. Sci. Farm., Univ. Genova, Genoa, I-16132, Italy
SOURCE: Farmaco (1993), 48(3), 335-55
CODEN: FRMCE8; ISSN: 0014-827X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

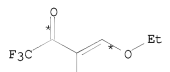


I

AB The synthesis of Et or Me 4-substituted or unsubstituted 2-methylthio-5-pyrimidinecarboxylates I (R = H or alkyl, R1 = Me or ethyl) mainly by reaction of Et or Me 2-dimethylaminomethylene-3-oxoalkanoates with 2-methylisothiourea is described. Also, some Et 2-substituted (NH2, CH3, C6H5) 4-trifluoromethyl-5-pyrimidinecarboxylates were prepared Some of the above esters were hydrolyzed to the relative carboxylic acids, which were decarboxylated to the corresponding 2,4-disubstituted pyrimidines. I were tested for their toxicity on Vero cultured cells and for their inhibitory activity against herpes simplex virus type 1 (HSV-1) infectivity in a short-term plaque assay. At non toxic concns., each ester was found to be active, the most interesting compound being I (R = benzyl, R' = ethyl), which achieved a 80.9% inhibition of HSV-1 infectivity at 12 μg/mL.

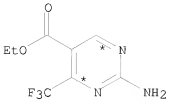
RX(11) OF 54 V + T ===> W...


V



T

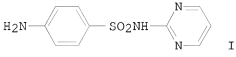
(11)



W
YIELD 68%

RX(11) RCT V 113-00-8, T 571-55-1
        PRO W 149771-09-5

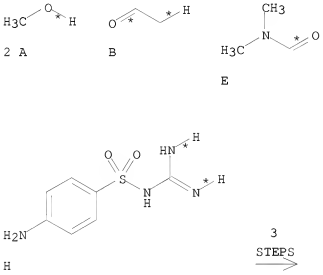
L3 ANSWER 28 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 119:117199 CASREACT
TITLE: Production of sulfadiazine from acetal
AUTHOR(S): Chen, Xiaochen
CORPORATE SOURCE: Shanghai Pharm. Ind. Assoc. Sales Dep., Shanghai, 200003, Peop. Rep. China
SOURCE: Zhongguo Yiyao Gongye Zazhi (1992), 23(12), 537-8
CODEN: ZYGZEA; ISSN: 1001-8255
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



I

AB Condensation of MeCH(OMe)2 with DMF in the presence of PCl3 gave Me2NCH:CHCH(OMe)2 which was treated with sulfaguanidine and NaOMe to give 85-91% the title compound (I).

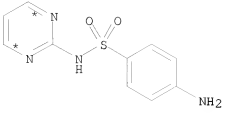
RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)
RX(6) 2 A + B + E + H ===> I



2 A B E

H

3 STEPS



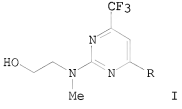
I
YIELD 91%

RX(1) RCT A 67-56-1, B 75-07-0
RGT D 10043-52-4 CaCl2
PRO C 534-15-6

RX(2) RCT E 68-12-2, C 534-15-6
RGT G 7719-12-2 PCl3
PRO F 1534-14-1

RX(3) RCT H 57-67-0, F 1534-14-1
RGT J 124-41-4 NaOMe
PRO I 68-35-9
SOL 67-56-1 MeOH

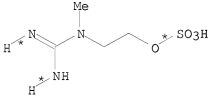
L3 ANSWER 29 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 119:28093 CASREACT
TITLE: New chemotherapeutically active of trifluoromethylpyrimidines
AUTHOR(S): Kreutzberger, Alfred; Burger, Angelika
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg Univ., Mainz, W-6500, Germany
SOURCE: Journal of Fluorine Chemistry (1993), 60(2-3), 257-61
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



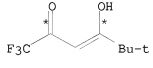
I

AB Condensation of N-(2-hydroxyethyl)-N-methylguanidine sulfate with various β-diketones bearing 1,1,1-trifluoromethyl substituents leads to 2-[N-(2-hydroxyethyl)-methylamino]-4-trifluoromethylpyrimidine derivs. I (R = Me, Et, CHMe2,CMe3). Compds. I exhibit antimycotic, trichomonazide and anti-HIV properties.

RX(1) OF 1 A + B ===> C

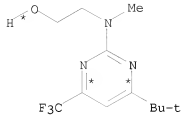


A



B

(1)



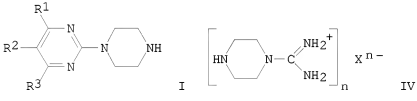
C
YIELD 38%

RX(1) RCT A 148191-13-3, B 74179-95-6
RGT D 497-19-8 Na2CO3
PRO C 148191-11-1
SOL 64-17-5 EtOH, 7732-18-5 Water

L3 ANSWER 30 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 117:151019 CASREACT
TITLE: Process for the preparation of piperazinylpyrimidine derivatives
INVENTOR(S): Kuo, David L.; Voeffray, Robert
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 491329	A1	19920624	EP 1991-121548	19911216
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
US 5204465	A	19930420	US 1991-803067	19911206
JP 04295467	A	19921020	JP 1991-330695	19911213
CA 2057782	A1	19920619	CA 1991-2057782	19911217
PRIORITY APPLN. INFO.:			CH 1990-4015	19901218
			CH 1991-639	19910304

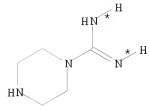
OTHER SOURCE(S): MARPAT 117:151019
GI



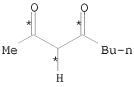
AB Title compds. I (R1, R2, R3 = H, C1-4 alkyl), useful as pharmaceutical intermediates, are prepared by acidifying piperazine (II) or its hydrate with cyanamide (III) to give piperazinylamidine salts IV (X = salt anion, n = charge of X) which, after optional isolation, are cyclized with 1,3-dicarbonyl compds. or their equivalent For example, reaction of II.6H2O with III in aqueous H2SO4 at 50-63° gave IV (X = SO4, n = 2) in 87.6% yield. Cyclization of this with (MeO)2CHCH2CH(OMe)2 in aqueous 50% H2SO4 at 70° gave, after workup and distillation in vacuo, 57% I (R1-R3 = H). Alternatively, reaction with 2,4-octanedione in NaOMe-HOMe at 80° to reflux gave 42% I (R1 = Me, R2 = H, R3 = Bu). Prepns. of addnl. I and precursors are described.

RX(1) OF 7 ...A + B ===> C

A: CM 1

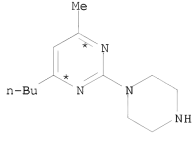


A: CM 2



B

(1)



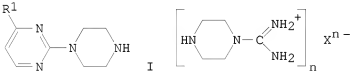
C
YIELD 42%

RX(1) RCT A 62122-69-4, B 14090-87-0
RGT D 124-41-4 NaOMe
PRO C 124863-75-8
SOL 67-56-1 MeOH
NTE reflux

L3 ANSWER 31 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 117:151018 CASREACT
TITLE: Process for the preparation of piperazinylpyrimidine derivatives
INVENTOR(S): Kuo, David L.
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 491328	A1	19920624	EP 1991-121547	19911216
EP 491328	B1	19960327		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
US 5200520	A	19930406	US 1991-804372	19911210
JP 04295468	A	19921020	JP 1991-330696	19911213
CA 2057751	A1	19920619	CA 1991-2057751	19911216
AT 136028	T	19960415	AT 1991-121547	19911216
ES 2084757	T3	19960516	ES 1991-121547	19911216

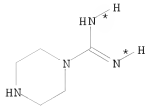
PRIORITY APPLN. INFO.: CH 1990-4014 19901218
OTHER SOURCE(S): MARPAT 117:151018
GI



AB Piperazinylpyrimidines I (R1 = H, C1-4 alkyl), useful as drug intermediates, are prepared by acidifying piperazine (II) or its hydrate with cyanamide (III) to give piperazinylamidine salts IV (X = salt anion, n = charge of X) which, after optional isolation, are cyclized with carbonyl compds. R1COCH:CHR2 [R2 = C1-4 alkoxy or (substituted) amino] in the presence of a base. For example, a mixture of II.6H2O, 95.6% H2SO4, and aqueous 25% III was stirred at 50° to give, after workup, 87.6% IV (n = 2, X = SO4). This was treated with NaOMe in MeOH, heated to reflux, and treated with Me2NCH:CHCHO to give, after workup and distillation in vacuo, 83% I (R1 = H). Using trans-MeOCH:CHCOMe in the 2nd step gave 53.9% I (R1 = Me).

RX(1) OF 5 ...A + B ===> C

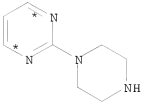
A: CM 1



A: CM 2

B

(1)



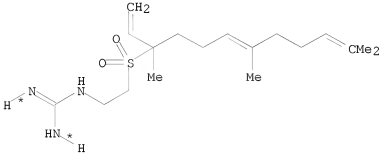
C
YIELD 83%

RX(1) RCT A 62122-69-4, B 927-63-9
RGT D 124-41-4 NaOMe
PRO C 20980-22-7
SOL 67-56-1 MeOH
NTE reflux

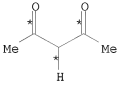
L3 ANSWER 32 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 117:90524 CASREACT
TITLE: Biomimetic synthesis of agelasidine A.
AUTHOR(S): Ichikawa, Yoshiyasu; Kashiwagi, Tikako; Urano, Noriko
CORPORATE SOURCE: Fac. Educ., Mie Univ., Tsu, 514, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (12), 1497-500
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Agelasidine A, (E)- MeC:CHCH2CH2CMe:CHCH2CH2CMe(CH:CH2)SO2CH2CH2NHC(NH2):NH, was synthesized using the [2,3]-sigmatropic rearrangement of allylic sulfinate, Me2C:CH(CH2CH2CMe:CH)2CH2OS(O)CH2CH2OAc, to an allylic sulfone at low concentration This biomimetic approach provided an efficient three-step synthesis of agelasidine A from farnesol in 54% overall yield.

RX(7) OF 26 ...B + W ===> X

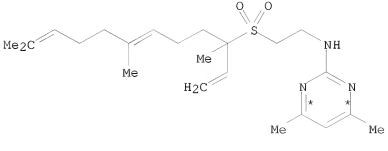


B



W

(7)



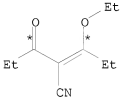
X
YIELD 28%

RX(7) RCT B 122566-13-6, W 123-54-6
PRO X 122619-94-7
SOL 110-86-1 Pyridine

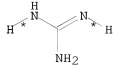
L3 ANSWER 33 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 117:69820 CASREACT
TITLE: Synthesis of 4,6-dialkylpyrimidine-5-carbonitriles
AUTHOR(S): McFadden, Helen G.; Huppatz, John L.
CORPORATE SOURCE: Div. Plant Ind., CSIRO, Canberra, 2601, Australia
SOURCE: Australian Journal of Chemistry (1992), 45(6), 1045-50
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 4,6-Dialkylpyrimidine-5-carbonitriles I (R, R' = Et, Me, Pr, Ph, CHMe2, X = S, O) were synthesized from 2-(1-ethoxyalkylidine)-3-oxoalkane-nitriles and bidentate nucleophiles such as thiourea in the presence of sodium ethoxide. The synthesis was found to be limited to dialkylpyrimidines where both alkyl groups contained between two and three carbons. Subsequent derivatization of the 2-thioxo function provides scope for the synthesis of a variety of novel pyrimidines.

RX(3) OF 3 A + J ===> K



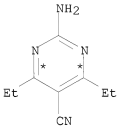
A



J: CM 1

J: CM 2

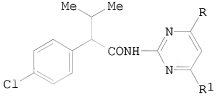
(3)



K
YIELD 50%

RX(3) RCT A 138134-00-6, J 593-85-1
PRO K 142673-60-7
SOL 64-17-5 EtOH

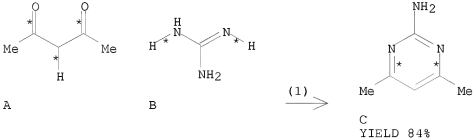
L3 ANSWER 34 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 114:185428 CASREACT
TITLE: Synthesis of amide-containing pyrimidines and their bioactivity
AUTHOR(S): Yu, Zhongsheng; Chen, Fuheng
CORPORATE SOURCE: Inst. Appl. Chem., Beijing Agric. Univ., Beijing, 100094, Peop. Rep. China
SOURCE: Yingyong Huaxue (1990), 7(6), 54-7
CODEN: YIHUED; ISSN: 1000-0518
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



I

AB Title compds. I (R = H, Me; R1 = Me, Ph, 4-FC6H4, 4-ClC6H4, 4-MeC6H4, 4-MeOC6H4) were prepared by amidation of 4-ClC6H4CH(CHMe2)COCl with aminopyridines. I (R = Me, R1 = 4-ClC6H4) was effective against Musca domestica and fungi.

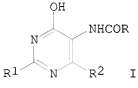
RX(1) OF 27 A + B ===> C...

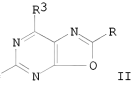


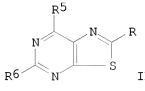
A B C
YIELD 84%

RX(1) RCT A 123-54-6, B 113-00-8
PRO C 767-15-7

L3 ANSWER 35 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 114:164148 CASREACT
TITLE: The synthesis of some thiazolo- and oxazolo[5,4-d]pyrimidines and pyrimidinylureas. II
AUTHOR(S): Hurst, Derek T.; Atcha, Shahid; Marshall, Kristina L.
CORPORATE SOURCE: Sch. Life Sci., Kingston Polytech., Kingston upon Thames/Surrey, KT1 2EE, UK
SOURCE: Australian Journal of Chemistry (1991), 44(1), 129-34
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

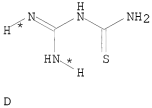

I

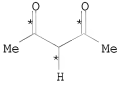

II


III

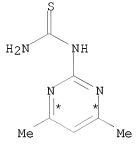
AB Acylamidopyrimidines I (R = H, Ph; R1 = H, SH, OH, SMe; R2 = H, OH, NH2) react with POCl3 or P2S5 to afford oxazolo[5,4-d]pyrimidines II (R3 = H, NH2, Cl, NHPOCl2; R4 = H, Cl, SMe) or thiazolo[5,4-d]pyrimidines III (R5 = H, NH2, SH; R6 = H, SH, SMe), resp. Thus, I (R= Ph, R1 = OH, R2 = H) treated with POCl3 gave 46% II (R3 = H, R4 = Cl) and with P2S5 gave 94% III (R5 = H, R6 = SH).

RX(2) OF 27 D + E ===> F...


D


E

(2)


F
YIELD 64%

RX(2) RCT D 2114-02-5, E 123-54-6
PRO F 88067-09-8

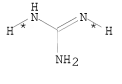
L3 ANSWER 36 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 114:102039 CASREACT
TITLE: Preparation of 2-amino-4,6-dimethylpyrimidine from guanidine and acetylacetone
INVENTOR(S): Liberovskaya, N. L.; Safina, F. G.; Bezsolitsen, V. P.; Promonenkov, V. K.; Sorokin, V. I.
PATENT ASSIGNEE(S): All-Union Scientific-Research Institute of Chemicals for Plant Protection, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1990, (29), 91-2. CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1583418	A1	19900807	SU 1988-4602939	19881014

PRIORITY APPLN. INFO.: SU 1988-4602939 19881014

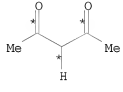
AB The title compound was prepared by addition of MeCOCH2COMe to a solution of guanidine sulfate in 53-76% H2SO4 (prepared in situ from cyanoguanidine and 75-94% H2SO2,) at 15-50° followed by neutralization with aqueous NH3.

RX(1) OF 3 ...A + B ===> C



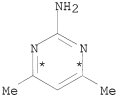
A: CM 1

A: CM 2



B

(1)

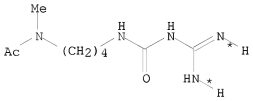


C
YIELD 93%

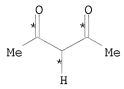
RX(1) RCT A 646-34-4, B 123-54-6
PRO C 767-15-7

L3 ANSWER 37 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 114:58885 CASREACT
TITLE: Nicaeensin, a new amidinoureido compound from the red alga Schottera nicaeensis
AUTHOR(S): Chillemi, Rosa; Morrone, Raffaele; Patti, Angela; Piattelli, Mario; Sciuto, Sebastiano
CORPORATE SOURCE: Dip. Sci. Chim., Univ. Catania, Catania, 95125, Italy
SOURCE: Journal of Natural Products (1990), 53(5), 1220-4
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
AB From the basic amino acid fraction of the red alga S. nicaeensis a previously reported nitrogenous compound was isolated by chromatog. and its structure determined as 1-(3-amidoureido)-4-(N-methylacetamido)butane (nicaeensin) by degradation and spectroscopic measurements.

RX(6) OF 6 A + H ===> I

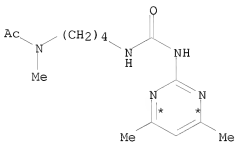


A



H

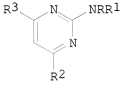
(6)



I

RX(6) RCT A 131669-98-2, H 123-54-6
PRO I 131670-02-5

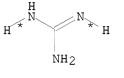
L3 ANSWER 38 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 113:115146 CASREACT
TITLE: Improved synthesis of fluoroalkyl and fluoroaryl substituted 2-aminopyrimidines
AUTHOR(S): Kucerovy, Andrew; Mattner, Paul G.; Hathaway, Joel S.; Repic, Oljan
CORPORATE SOURCE: Sandoz Pharm. Corp., East Hanover, NJ, 07936, USA
SOURCE: Synthetic Communications (1990), 20(6), 913-17
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

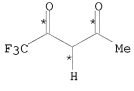
AB Aminopyrimidines I (R = R1 = H,Me; R = H, R1 = Et; R2 = CF3, R1 = Me, Ph, 2-thienyl; R2 = 4-FC6H4, R3 = Me2CH) were prepared by cyclization of guanidine RR1NC(NH)NH2 salts with fluorine-substituted β-diketones R2COCH2COR3 in Me2CHONa/Me2CHOH at reflux.

RX(1) OF 1 A + B ===> C



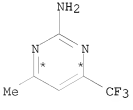
A: CM 1

A: CM 2



B

(1)



C
YIELD 90%

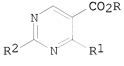
RX(1) RCT A 594-14-9

```
   STAGE(1)
      RGT  D 7440-23-5 Na
      SOL  67-63-0 Me2CHOH

   STAGE(2)
      RCT  B 367-57-7
      SOL  67-63-0 Me2CHOH

PRO  C 5734-63-4
```

L3 ANSWER 39 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 113:40613 CASREACT
TITLE: Reaction of 2-dimethylaminomethylene-1,3-diones with dinucleophiles. VIII. Synthesis of ethyl and methyl 2,4-disubstituted 5-pyrimidinecarboxylates
AUTHOR(S): Schenone, Pietro; Sansebastiano, Laura; Mosti, Luisa
CORPORATE SOURCE: Ist. Sci. Farm., Univ. Genova, Genoa, 16132, Italy
SOURCE: Journal of Heterocyclic Chemistry (1990), 27(2), 295-305
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

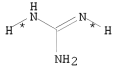


I

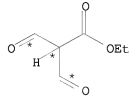
AB Cyclocondensation of HOCH:C(CHO)CO2Et or Me2NCH:C(CO2R)COR1 (R = Me, Et; R1 = H, Me, Et, Pr, CHMe2, CMe3, CH2Ph, Ph) with HN:CR2NH2 (R2 = NH2, Me, Ph) gave the title compds. I in 22-88% yield. I were then hydrolyzed to the corresponding acids followed by decarboxylation.

RX(1) OF 149 A + B ===> C...

A: CM 1

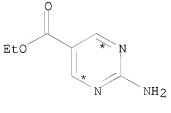


A: CM 2



B

(1)

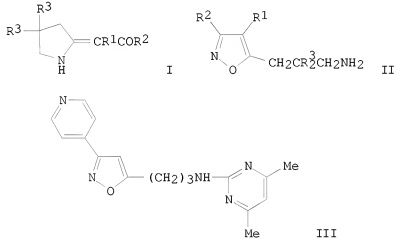


C
YIELD 35%

RX(1) RCT A 593-87-3, B 80370-42-9
RGT D 141-52-6 NaOEt

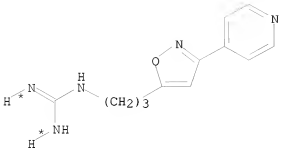
PRO C 57401-76-0
SOL 64-17-5 EtOH

L3 ANSWER 40 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 112:178745 CASREACT
TITLE: Ring transformations of phenacylidenepyrrolidines. Synthesis of 5-(3-aminopropyl)isoxazoles
AUTHOR(S): Dannhardt, Gerd; Obergrusberger, Irmengard
CORPORATE SOURCE: Inst. Pharm. Chem., Johann Wolfgang Goethe-Univ., Frankfurt/Main, Fed. Rep. Ger.
SOURCE: Chemiker-Zeitung (1989), 113(6), 220-2
CODEN: CMKZAT; ISSN: 0009-2894
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

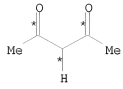


AB Ring transformation of phenacylidene pyrrolidines with NH2OH·HCl yields aryl-, diaryl- and heteroaryl-isoxazoles with an amino-Pr side chain at position C-5. The reaction mechanism is discussed, all new compds. are characterized by spectrometric methods. Thus, reaction of phenacylidenepyrrolidines I [R1 = H, R2 = 4-MeC6H4, 4-H2NC6H4, 4-HOC6H4, 4-C6H4C(NH2):NOH, R3 = Me; R1 = H, R2 = 4-pyridinyl, Ph, R3 = H; R1 = Ph, R2 = Ph, 4-pyridinyl, R3 = Me] with NH2OH·HCl in MeOH-H2O containing NaOAc gave 49-74% aminopropylisoxazoles II. Amination of II (R1 = H, R2 = 4-pyridinyl, R3 = H) with dimethylguanidinopyrazole nitrate followed by cyclization with MeCOCH2COMe gave pyrimidine III.

RX(10) OF 13 ...V + Y ===> Z

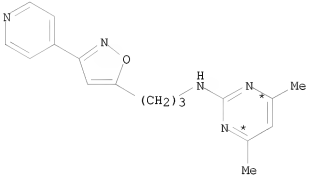


V



Y

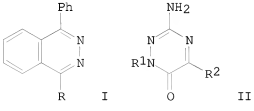
(10)



Z
YIELD 64%

RX(10) RCT V 126381-58-6, Y 123-54-6
RGT AA 584-08-7 K2CO3
PRO Z 126381-59-7
SOL 64-17-5 EtOH

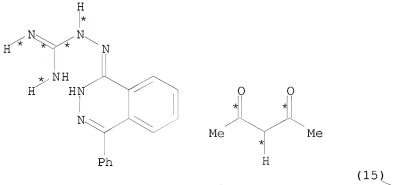
L3 ANSWER 41 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 112:118743 CASREACT
TITLE: Synthesis and reactions of phthalazine derivatives. Part III. Synthesis of heterocyclic compounds containing the 4-phenylphthalazin-1-yl moiety as fungicidal agents
AUTHOR(S): El-Gendy, Z.; Abdel-Rahman, R. M.; Abdel-Malik, M. S.
CORPORATE SOURCE: Fac. Educ., Ain-Shams Univ., Cairo, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1989), 28B(6), 479-85
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



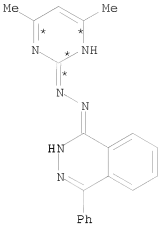
I II

AB A number of heterocyclic systems bearing 4-phenylphthalazin-1-yl moiety have been synthesized by interaction of 1-(4-phenylphthalazin-1-ylamino)guanidine and thiosemicarbazide with α,β-bifunctional compds. in neutral or alkaline medium. Some of them, e.g. I [R = NHN:C(NH2)2, NHNHCSNH2] or dihydrotriazines II (R1 = 4-phenylphthalazin-1-yl, R2 = 2-O2NC6H4, Et, PhCH2), have been evaluated for their antifungal activity against Aspergillus niger and Penicillum oxalicum.

RX(15) OF 57 A + AG ===> AH



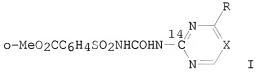
A AG (15)



AH

RX(15) RCT A 125706-69-6, AG 123-54-6
PRO AH 125706-83-4
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH

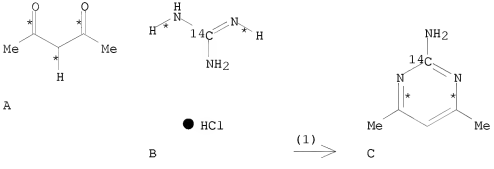
L3 ANSWER 42 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 112:35813 CASREACT
TITLE: Synthesis of [14C]-sulfometuron-methyl and [14C]-metsulfuron-methyl
AUTHOR(S): Bastide, Jean; Badon, Robert
CORPORATE SOURCE: Univ. Perpignan, Perpignan, 66025, Fr.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1989), 27(6), 715-20
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



I

AB Title compds. I (X = N, R = OMe; X = CH, R = Me) were prepared from H2N14CN and HN:14C(NH2)2.HCl, resp. The key step was acylation of the appropriate amino heterocycle with o-MeO2CC6H4SO2NCO.

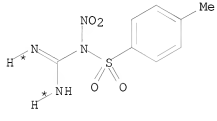
RX(1) OF 15 A + B ===> C...



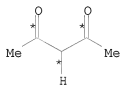
RX(1) RCT A 123-54-6, B 73549-39-0
RGT D 497-19-8 Na2CO3
PRO C 124475-81-6
SOL 7732-18-5 Water

L3 ANSWER 43 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 111:194249 CASREACT
TITLE: Synthesis and properties of isomeric N-arylsulfonyl-N-nitroguanidines
AUTHOR(S): Dobronravov, A. N.; Svistun, N. V.; Dubina, V. L.
CORPORATE SOURCE: Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1989), 25(3), 536-9
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB N-Tosyl-N-nitroguanidines with the nitro-group on different N atoms, e.g., TsNHC(NH2):NNO2, Ts(O2N)NC(NH2):NH, were prepared and their reactions with CH2N2, MeCOCH2COMe, amines, and alkaline hydrolysis studied.

RX(4) OF 17 ...F + M ===> N

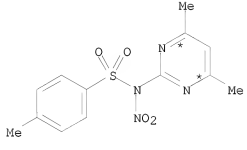


F



M

(4)



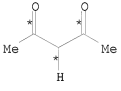
N
YIELD 82%

RX(4) RCT F 90953-34-7, M 123-54-6
RGT O 64-19-7 AcOH
PRO N 123458-64-0

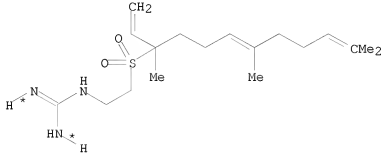
L3 ANSWER 44 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 111:154141 CASREACT
TITLE: First synthesis of agelasidine A
AUTHOR(S): Ichikawa, Yoshiyasu
CORPORATE SOURCE: Fac. Educ., Mie Univ., Tsu, 514, Japan
SOURCE: Tetrahedron Letters (1988), 29(39), 4957-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of Me2C:CHCH2CH2CMe:CHCH2CH2CMe(CH:CH2)SO2CH2CH2NHC(:NH)NH2 (I) was accomplished in 8 steps starting from farnesol. The quaternary C of I was constructed by the hetero-Claisen rearrangement of Me2C:CHCH2CH2CMe:CHCH2CH2CMe:CHCH2OCS2Me. This methodol. provides the basis for a general and efficient route to the agelasidinine skeleton.

RX(1) OF 36 ...A + B ===> C

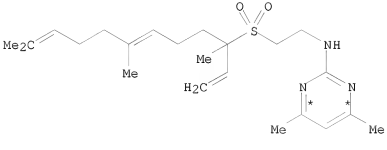


A



B

(1)



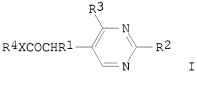
C

RX(1) RCT A 123-54-6, B 122566-13-6
RGT D 110-86-1 Pyridine
PRO C 122619-94-7

L3 ANSWER 45 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 111:153826 CASREACT
TITLE: Preparation of pyrimidine-containing carboxylic acid esters having insecticidal and acaricidal activities
INVENTOR(S): McDonald, Edward; Salmon, Roger; Whittle, Alan John; Hutchings, Michael Gordon
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Eur. Pat. Appl., 104 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 295839	A2	19881221	EP 1988-305337	19880610
EP 295839	A3	19910731		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 8803862	A	19890222	ZA 1988-3862	19880530
AU 8817389	A	19881222	AU 1988-17389	19880603
AU 610184	B2	19910516		
GB 2209525	A	19890517	GB 1988-13780	19880610
GB 2209525	B	19910403		
HU 47384	A2	19890328	HU 1988-3052	19880615
HU 203644	B	19910930		
BR 8802952	A	19890110	BR 1988-2952	19880616
DK 8803348	A	19881218	DK 1988-3348	19880617
CN 1030412	A	19890118	CN 1988-103836	19880617
CN 1019574	B	19921223		
JP 01016769	A	19890120	JP 1988-148425	19880617
SU 1801108	A3	19930307	SU 1988-4613066	19881212

PRIORITY APPLN. INFO.: GB 1987-14233 19870617
OTHER SOURCE(S): MARPAT 111:153826
GI

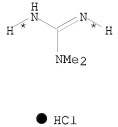


I

AB The title compds. [I; R1 = C1-6 alkyl, C2-8 alkenyl, C2-6 alkynyl, C1-4 haloalkyl, C2-8 haloalkenyl, C3-6 cycloalkyl optionally substituted by ≥1 C1-4 alkyl or halo; R2 = C1-8 alkyl, C1-4 haloalkyl, C1-6 alkoxy, halo, C3-6 cycloalkyl optionally substituted by ≥1 C1-4 alkyl or halo, Ph optionally substituted by ≥1 C1-4 alkyl, C1-4 haloalkyl, or C1-4 alkoxy; R3 = H, halo; R4 = residue of an alc. of formula R4-OH which forms an insecticidal ester when combined with chrysanthemic acid, permethrin, or cyhalothrin acid; X = O, S], useful as insecticides or acaricides, were prepared To a stirred solution of 0.1 (RS)-2-[2-(1,1-dimethylethyl)pyrimidin-5-yl]-3,3-dimethylbutanoic acid, 0.089 2,3,5,6-tetrafluoro-4-(methoxymethyl)benzyl alc., and 0.002 g 4-dimethylaminopyridine in CH2Cl2, 0.084 g DCC was added and the mixture was

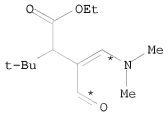
stirred 18 h to give 0.09 g 2,3,5,6-tetrafluoro-4-(methoxymethyl)benzyl (RS)-2-[2-(1,1-dimethylethyl)pyrimidin-5-yl]-3,3-dimethylbutanoate (II). II at 500 ppm gave 50-79% mortality against Blattella germanica and 80-100% mortality against 9 addnl. pest species, e.g. Tetranychus urticae, Nephotettix cinticeps, and Diabrotica balteata. An emulsifiable concentrate composition containing Synperonic OP10 3.0, calcium dodecylbenzenesulfonate 2.0,
and Aromasol H 94.0 weight % was prepared

RX(34) OF 322 ...BW + BM ===> BX



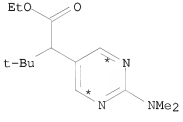
● HCl

BW



BM

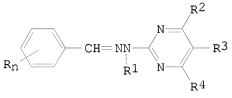
(34)



BX

RX(34) RCT BW 22583-29-5, BM 122936-12-3
PRO BX 122936-22-5
CAT 141-52-6 NaOEt

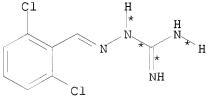
L3 ANSWER 46 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 111:148707 CASREACT
TITLE: Studies on fungicidal pyrimidinylhydrazones. I. Fungicidal activity of aromatic aldehyde pyrimidinylhydrazones
AUTHOR(S): Konishi, Kazuo; Kuragano, Takashi; Tsujikawa, Teruaki
CORPORATE SOURCE: Agro Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan
SOURCE: Nippon Noyaku Gakkaishi (1989), 14(2), 189-96
CODEN: NNGADV; ISSN: 0385-1559
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



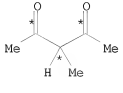
I

AB Pyrimidinylhydrazones (I, R = H, Cl, anthryl, SCH2Ph, Me, etc.; R1 = H, Ac, Me; R2 = Me, H; R3 = H, Me, Et; R4 = H, alkyl, CF3, Cl, MeO, EtO; n = 1-4) were prepared by the condensation of aromatic aldehydes with pyrimidinylhydrazines or by the reaction of aralkylideneaminoguanidines with β-dicarbonyl compds. and their fungicidal activity against Pyricularia oryzae, Helminthosporium oryzae and H. sigmoideum irregulare related to their structures. Aryl and other heteroarylhydrazones were also prepared and their fungicidal activity compared with I. A pyrimidinylhydrazone function was a requisite for fungicidal activity, as shown by the loss of activity when 2-pyrimidinylhydrazine was replaced by aromatic or other heteroarom. hydrazines. Covering the hydrazine proton by N-acetylation or N-methylation did not attenuate the activity. Steric congestion near the hydrazone bond increased activity.

RX(2) OF 2 D + E ===> C

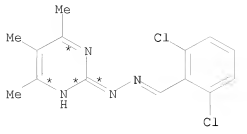


D



E

(2)



C

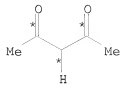
RX(2) RCT D 5051-62-7, E 815-57-6
PRO C 66957-89-9

L3 ANSWER 47 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 111:134755 CASREACT
TITLE: Preparation of decapeptides as LHRH antagonists having high antiovulatory activity and negligible histamine releasing activity
INVENTOR(S): Folkers, Karl; Bowers, Cyril Y.; Ljungquist, Anders; Tang, Pui Fun Louisa; Kobota, Minoru; Feng, Dong Mei
PATENT ASSIGNEE(S): University of Texas System, USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

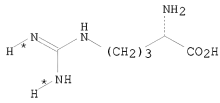
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8901944	A1	19890309	WO 1988-US2922	19880824
W: AT, AU, BB, BG, BR, CH, DE, DK, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU, US				
RW: AT, BE, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
US 4935491	A	19900619	US 1987-88431	19870824
AU 8825294	A	19890331	AU 1988-25294	19880824
AU 619221	B2	19920123		
EP 377665	A1	19900718	EP 1988-908786	19880824
EP 377665	B1	19950712		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 03501969	T	19910509	JP 1988-507982	19880824
HU 59940	A2	19920728	HU 1988-5868	19880824
HU 213098	B	19970228		
CA 1339659	C	19980203	CA 1988-587364	19881230
KR 135276	B1	19980423	KR 1989-700699	19890421
DK 9000486	A	19900419	DK 1990-486	19900223
DK 173753	B1	20010910		
NO 9000888	A	19900423	NO 1990-888	19900223
NO 301015	B1	19970901		
FI 102074	B1	19981015	FI 1990-947	19900223
NO 9402179	A	19900423	NO 1994-2179	19940610
NO 302577	B1	19980323		
PRIORITY APPLN. INFO.:			US 1987-88431	19870824
			WO 1988-US2922	19880824
			NO 1990-888	19900223

AB Decapeptide analogs of LHRH, e.g. [N-Ac-D-2-Nal1, D-pClPhe2, D-3-Pal3, NicLys5, D-NicLys6, Ilys8, D-Ala10]-LHRH [2-Nal = 3-(2-naphthyl)alanine, pClPhe = 3-(4-chloro)phenylalanine, 3-Pal = 3-(3-pyridyl)alanine, NicLys = Nε-anisotinoy l, Ilys = Nε-isopropyllysine] (I) (Antide) having high ovulation inhibition activity and very low histamine release activity, were prepared I and other decapeptides were synthesized by the solid phase method using a Beckman Model 990 peptide synthesizer, new lysine, ornithine, alanine, glutamic acid and arginine derivs., and benzhydrylamine hydrochloride resin as a solid support. I showed antiovulatory activity (AOA) of 100% at 1 μg and 36% at 0.5 μg in rats and an ED50 of ≥300 μg/mL for histamine release in a rat mast cell assay.

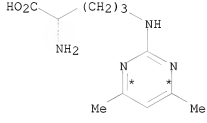
RX(1) OF 21 A + B ===> C...



A



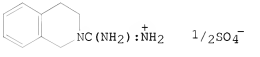
B



C

RX(1) RCT A 123-54-6, B 1119-34-2
RGT D 144-55-8 NaHCO3
PRO C 55684-38-3

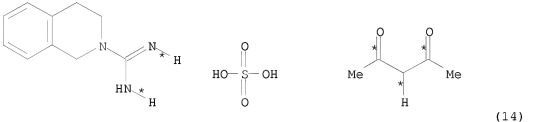
L3 ANSWER 48 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 110:212577 CASREACT
TITLE: Synthesis of deuterated 1,2,3,4-tetrahydroisoquinolines
AUTHOR(S): Meese, Claus O.; Ebner, Thomas
CORPORATE SOURCE: Dr. Margarete Fischer-Bosch-Inst. Klin. Pharmakol., Stuttgart, D-7000/50, Fed. Rep. Ger.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(3), 335-43
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



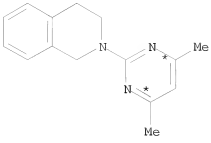
I

AB 1,2,3,4-Tetrahydroquinolines, either randomly or regioselectively (1,1-D2, 3,3-D2, 4,4-D2) labeled with D, were prepared from isoquinoline, 2-indanone, and PhCH2CN. The deuterated bases were used in preparation of labeled analogs of the hypertensive agent debrisoquine (I).

RX(14) OF 94 AP + AQ ===> AR



AP: CM 1 AP: CM 2 AQ



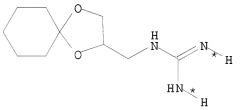
AR
YIELD 80%

RX(14) RCT AP 581-88-4, AQ 123-54-6
        RGT AS 144-55-8 NaHCO3
        PRO AR 120507-37-1
        SOL 7732-18-5 Water, 108-88-3 PhMe

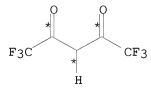
L3 ANSWER 49 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 110:107483 CASREACT
TITLE: Gas-chromatographic determination of guanadrel in plasma and urine
AUTHOR(S): Kaiser, David G.; Vangiessen, Garrett J.; Shah, Jyoti A.; Weber, Dennis J.
CORPORATE SOURCE: Drug Metab. Res., Upjohn Co., Kalamazoo, MI, 49001, USA
SOURCE: Journal of Chromatography (1988), 434(1), 135-43
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To evaluate the pharmacokinetics and drug availability from various dosage formulations, a method for the determination of guanadrel in plasma and urine was required. A gas-chromatog. procedure, based on formation of a hexafluoroacetylacetone derivative in a 2-phase system of H2O and PhMe, was developed. The limit of determination of the method is 5 ng guanadrel/mL plasma and 15 ng/mL urine. Statistical analyses indicated average recoveries of 98.1 and 10.4.4% from plasma and urine, resp. Mass-spectrometric analyses, in conjunction with gas chromatog., confirmed the specificity of the method for intact drug. The procedure was applied successfully to drug absorption studies in humans.

RX(1) OF 2 A + B ===> C

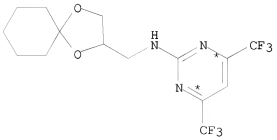


A



B

(1)



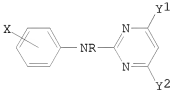
C

RX(1) RCT A 40580-59-4, B 1522-22-1
PRO C 119386-80-0

L3 ANSWER 50 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 109:124400 CASREACT
TITLE: Preparation of pyrimidine derivatives as fungicides
INVENTOR(S): Shigekazu, Ito; Katsumi, Masuda; Shoji, Kusano; Toshihiro, Nagata; Yoshiyuki, Kojima; Nobumitsu, Sawai; Shinichiro, Maeno
PATENT ASSIGNEE(S): Kumiai Chemical Industry Co., Ltd., Japan; Ihara Chemical Industry Co., Ltd.
SOURCE: Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 270111	A1	19880608	EP 1987-117893	19871203
EP 270111	B1	19910515		
R: CH, DE, FR, GB, IT, LI, NL				
JP 63141971	A	19880614	JP 1986-288247	19861203
JP 07084445	B	19950913		
US 4992438	A	19910212	US 1990-512901	19900420
PRIORITY APPLN. INFO.:			JP 1986-288247	19861203
			US 1987-127426	19871202

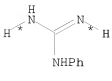
OTHER SOURCE(S): MARPAT 109:124400
GI



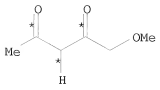
I

AB The pyrimidines I (X = H, halo, alkyl, alkoxy, haloalkyl, CN; Y1 = alkyl, cyanoalkyl, alkoxy, alkenyl, alkynyl, etc.; Y2 = halo, alkyl, haloalkyl; R = H, alkyl, NO, alkoxyalkyl, alkenyl, etc.; substituents are subject to restrictions) are prepared as fungicides. 2-Anilino-4-methyl-6-(1-propynyl)pyrimidine was added to a suspension of NaH in THF, followed by the addition of ClCH2OMe, to give I (Y1 = C.tplbond.CMe, Y2 = Me, X = H, R = CH2OMe) (II). II (500 ppm) prevented artificial infection of rice with Pyricularia oryzae blast. A wettable powder was made of II 50, diatomaceous earth 45, Na dinaphthylmethanesulfonate 2, and Na ligninsulfonate 3%.

RX(1) OF 20 A + B ===> C...

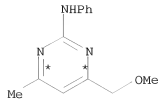


A



B

(1)



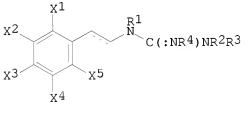
C
YIELD 68%

RX(1) RCT A 2002-16-6, B 6290-50-2
RGT D 497-19-8 Na2CO3
PRO C 116389-17-4

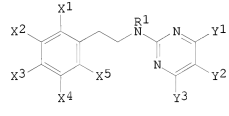
L3 ANSWER 51 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 109:104790 CASREACT
TITLE: Antiviral guanidine derivative compositions and their methods of use
INVENTOR(S): Higa, Tatsuo; Sakai, Ryuichi
PATENT ASSIGNEE(S): Harbor Branch Oceanographic Institution, Inc., USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8800181	A1	19880114	WO 1987-US1562	19870625
W: JP				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
US 4772609	A	19880920	US 1986-879079	19860626
EP 271571	A1	19880622	EP 1987-904612	19870625
R: DE, FR, GB, IT				
JP 01500518	T	19890223	JP 1987-504279	19870625
US 4851441	A	19890725	US 1988-153469	19880128
PRIORITY APPLN. INFO.:			US 1986-879079	19860626
			WO 1987-US1562	19870625

OTHER SOURCE(S): MARPAT 109:104790
GI



I

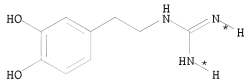


II

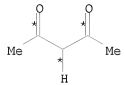
AB Guanidine derivs. I and II [R1-R4 = H, OH, acyl, alkyl; X1-X5, Y1-Y3 = H, OH, SH, NO2, alkylthio, (mono- or dialkyl)amino, alkylsulfonyl, aminosulfonyl, hydroxysulfonyl, acylamino, halo, alkoxy, acyloxy] from corals (Tubastrea aurea) are useful for control of viral diseases in animals and plants. Tubastrine (I; X1, X2, X5, R1-R4 = H; X3, X4 = OH; double bond) (III) was extracted from T. aurea with Me2CO, partitioned between EtOAc and H2O, and purified by chromatog. on polystyrene gel, silica gel,

TSK HW-40, and Sephadex LH-20. Purified III was converted to the tetraacetate, diacetate, dihydro derivative, and II. III at 200 μg/0.5 mL completely inhibited vesicular stomatitis virus and herpes simplex virus 1 in CV-1 fibroblast-like cells in vitro.

RX(1) OF 1 A + B ===> C

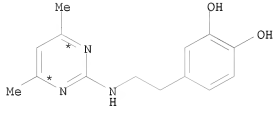


A



B

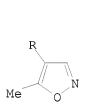
(1)



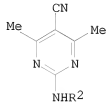
C

RX(1) RCT A 78406-92-5, B 123-54-6
PRO C 107585-48-8

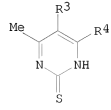
L3 ANSWER 52 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 107:77747 CASREACT
TITLE: Base-induced ring cleavage of 4-functionalized 3-unsubstituted isoxazoles. Synthesis of 2-aminopyrimidines and pyrimidine-2(3H)-thiones
AUTHOR(S): Alberola, Angel; Antolin, Luis F.; Gonzalez, Ana M.; Laguna, Miguel A.; Pulido, Francisco J.
CORPORATE SOURCE: Dep. Quim. Org., Univ. Valladolid, Valladolid, Spain
SOURCE: Heterocycles (1987), 25(1), 393-7
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



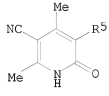
I



II



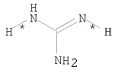
III



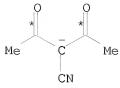
IV

AB 4-Functionalized 3-unsubstituted isoxazoles I (R = Ac, NO2) undergo ring cleavage when treated with bases. The resulting open chain products (β-cyanoenolates RC(CN):CMeONa, β-enaminonitriles RC(CN):CMeNHR1, R1 = Me, Ph) were converted into pyrimidines, II (R2 = H, Me) pyrimidinethiones III (R3 = NO2, cyano; R4 = Me, NH2) and pyridinones IV (R5 = CO2H, cyano) by reaction with 1,3-dinucleophiles (guanidine, thiourea) and compds. having activated methylene groups.

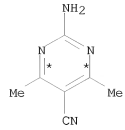
RX(1) OF 16 A + B ===> C



A



B



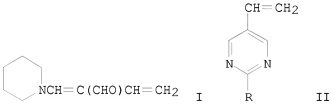
C

(1)

YIELD 17%

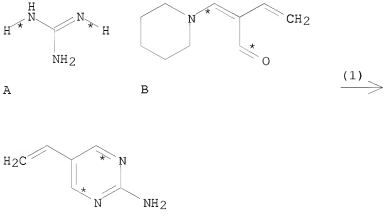
RX(1) RCT A 113-00-8, B 22466-40-6
PRO C 16341-54-1
SOL 64-17-5 EtOH

L3 ANSWER 53 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:213887 CASREACT
TITLE: A new synthesis of 5-vinylpyrimidines
AUTHOR(S): Kvita, Vratislav
CORPORATE SOURCE: Zent. Forschungslab., Ciba-Geigy A.-G., Basel, CH-4002, Switz.
SOURCE: Synthesis (1986), (9), 786-8
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Cyclization of piperidylacrolein I with amidines RC(:NH)NH2 [R = NH2, NMe2, CH2CHMe2, p-tolyl, m-F3CC6H4, o-ClC6H4, p-[Me(CH2)7]C6H4, p-O2NC6H4, 3,5-(O2N)2C6H3, 1-naphthyl, 2-pyridyl, 2-pyridyl, 2-pyrimidyl, 4,6-dimethyl-2-pyrimidyl] gave 22-78% title compds. II.

RX(1) OF 13 A + B ===> C



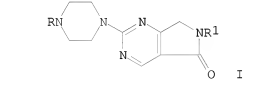
A B C
YIELD 78%

RX(1) RCT A 113-00-8, B 85438-16-0
PRO C 108444-56-0
SOL 75-05-8 MeCN, 67-56-1 MeOH

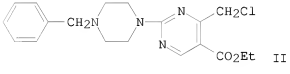
L3 ANSWER 54 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:176420 CASREACT
TITLE: 2-Piperazinopyrimidines
INVENTOR(S): Yokoyama, Keiichi; Ono, Hiroyasu; Kato, Sukishige; Kitahara, Takumi
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61243082	A	19861029	JP 1985-84455	19850422
JP 06035460	B	19940511		

PRIORITY APPLN. INFO.: JP 1985-84455 19850422
GI



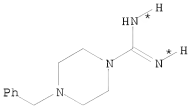
I



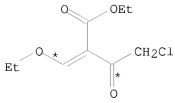
II

AB Title compds. I [R = H, aralkyl; R1 = (substituted) alkyl, aralkyl, cycloalkyl], useful as herbicides (no data), were prepared Thus, treating 9.7 g 1-amidino-4-benzylpiperazine H2SO4 salt with 1.5 g NaOH and then 8 g ClCH2COC(:CHOEt)CO2Et gave 86.7% II, 2 g of which was then refluxed with 10.5 g cyclohexylamine in isoamyl alc. to give 63% I (R = PhCH2, R1 = cyclohexyl).

RX(1) OF 11 A + B ===> C...

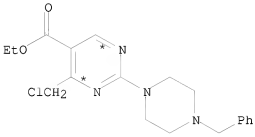


A



B

(1)



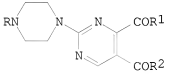
C

RX(1) RCT A 7773-69-5, B 91168-75-1
PRO C 104966-06-5

L3 ANSWER 55 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:102320 CASREACT
TITLE: 2-Piperazinopyrimidines
INVENTOR(S): Yokoyama, Keiichi; Ono, Hiroyasu; Kato, Sukishige; Kitahara, Takumi
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61243067	A	19861029	JP 1985-82522	19850419
JP 06000764	B	19940105		
PRIORITY APPLN. INFO.:			JP 1985-82522	19850419

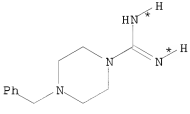
GI



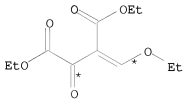
I

AB Title compds. (I; R = H, aralkyl; R1, R2 = alkoxy, OH, alkylamino; R1R2 = alkyl-substituted imino group), useful as herbicides (no data), were prepared Thus, treating 1-amidino-4-benzylpiperazine 1/2 H2SO4 salt with EtO2CCOC(CO2Et):CHOEt in the presence of NaOEt at room temperature for 2 days gave 96% I (R = PhCH2, R1 = R2 = OEt).

RX(1) OF 3 A + B ===> C...

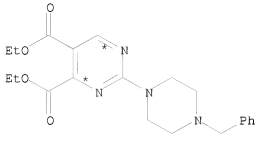


A



B

(1)



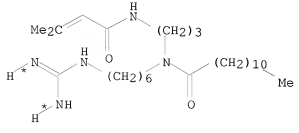
C

RX(1) RCT A 7773-69-5, B 52942-64-0
PRO C 104966-59-8

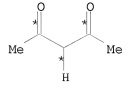
L3 ANSWER 56 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:66978 CASREACT
TITLE: Synthesis of acarnidines: guanidinated spermidine homologs through imine intermediates
AUTHOR(S): Yorke, Selwyn C.; Blunt, John W.; Munro, Murray H. G.; Cook, J. Carter; Rinehart, Kenneth L., Jr.
CORPORATE SOURCE: Dep. Chem., Univ. Canterbury, Christchurch, N. Z.
SOURCE: Australian Journal of Chemistry (1986), 39(3), 447-55
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English

AB One of the naturally occurring acarnidines, Me2C:CHCONH(CH2)nN(COR)(CH2)mNHC(:NH)NH2[I, n = 3, m = 5, R = (CH2)10Me] and together with 17 analogs I[n = 2,3,5; m = 2,4-6; R = Me, (CH2)10Me,(CH2)16Me, (Z)-(CH2)7CH:CH(CH2)7Me] were prepared via reaction of Me2C:CHCONH(CH2)n-1CHO with H2N(CH2)mNH = CO2CMe3 and incorporation of the guanidine function in the last step.

RX(75) OF 430 ...CS + CX ===> CY

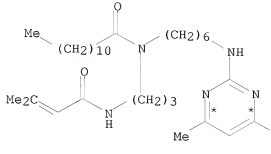


CS



CX

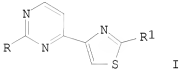
(75)



CY

RX(75) RCT CS 106491-14-9, CX 123-54-6
RGT CZ 497-19-8 Na2CO3
PRO CY 106491-19-4
SOL 7732-18-5 Water, 64-17-5 EtOH

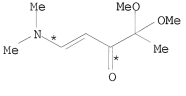
L3 ANSWER 57 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:32965 CASREACT
TITLE: 2-Amino- and 2-guanidino-4-thiazolylpyrimidines
AUTHOR(S): Lipinski, Christopher A.; Craig, Rebecca H.; Wright, Roger B.
CORPORATE SOURCE: Cent. Res., Pfizer, Inc., Groton, CT, 06340, USA
SOURCE: Journal of Heterocyclic Chemistry (1985), 22(6), 1723-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

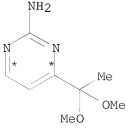
AB Synthesis of the four amino- and guanidinothiazolylpyrimidines I [R,R1 = NH2, NHC(:NH)NH2] is described and pKa values are calculated Guanidinopyrimidines are more basic than guanidinothiazoles. However, the reverse is true of the amino heterocycles; the aminothiazole is more basic than the aminopyrimidine.

RX(3) OF 31 ...G ===> A...



G

(3)



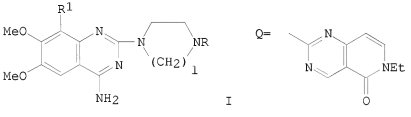
A
YIELD 76%

RX(3) RCT G 106157-94-2
RGT H 141-52-6 NaOEt, I 50-01-1 Guanidine chloride
PRO A 106157-85-1
SOL 64-17-5 EtOH

L3 ANSWER 58 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:18629 CASREACT
TITLE: 4-Amino-6,7-dimethoxyquinazoline derivatives
INVENTOR(S): Yokoyama, Keiichi; Kato, Koji; Kitahara, Takumi; Ono, Hiroyasu; Nishina, Takashi; Kumakura, Mikio; Awaya, Akira; Nakano, Takuo
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan; Mitsui Pharmaceuticals, Inc.
SOURCE: Jpn. Kokai Tokkyo Koho, 56 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61140568	A	19860627	JP 1984-263015	19841214
JP 05028709	B	19930427		
US 4734418	A	19880329	US 1985-805905	19851206
CA 1307786	C	19920922	CA 1985-497106	19851206
EP 188094	A2	19860723	EP 1985-309049	19851212
EP 188094	A3	19871223		
EP 188094	B1	19920318		
R: DE, FR, GB, IT				
HU 42479	A2	19870728	HU 1985-4783	19851213
HU 198481	B	19891030		
PRIORITY APPLN. INFO.:			JP 1984-263015	19841214
			JP 1985-194968	19850905
			JP 1985-204463	19850918

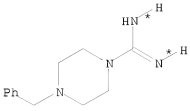
GI



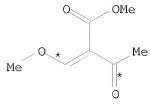
I

AB The title compds. (I; R = heterocyclyl; R1 = H, MeO; l = 2, 3), useful as antihypertensives, were prepared Thus, a mixture of 4-amino-2-chloro-6,7-dimethoxyquinazoline and 5,6-dihydro-6-ethyl-5-oxo-2-piperazinopyrido[4,3-d]pyrimidine in Me2CHCH2CH2OH containing Et3N was refluxed for 4 h to give 83% I (R = Q; R1 = H; l = 2). I at 1 mg/kg p.o. lowered the blood pressure in spontaneously hypertensive rats. Tablets containing I were prepared

RX(2) OF 52 C + D ===> E...

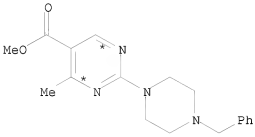


C



D

(2)

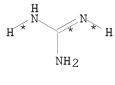


E

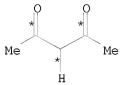
RX(2) RCT C 7773-69-5, D 58700-99-5
PRO E 102976-03-4

L3 ANSWER 59 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:225542 CASREACT
TITLE: A carbon-13 nuclear magnetic resonance study of the pyrimidine synthesis by the reactions of 1,3-dicarbonyl compounds with amidines and ureas
AUTHOR(S): Katritzky, Alan R.; Yousaf, Taher I.
CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
SOURCE: Canadian Journal of Chemistry (1986), 64(10), 2087-93
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The detailed mechanistic pathways are elucidated for the reactions of acetylacetone, Me acetonate, and di-Me malonate with a variety of amidines and ureas. In many cases the identification of a single intermediate allows the definition of the reaction path and identification of two slow steps. Intermediates characterized include ring-closed dihydroxytetrahydropyrimidines, dihydrohydroxypyrimidinones, open-chain enamides, and carbonyl addition compds.

RX(1) OF 37 A + B ===> C...

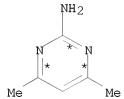


A



B

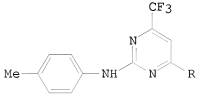
(1)



C

RX(1) RCT A 113-00-8, B 123-54-6
PRO C 767-15-7
SOL 2206-27-1 DMSO-d6

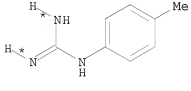
L3 ANSWER 60 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:133828 CASREACT
TITLE: Antidiabetic substances. IV. Trifluoromethyl-2-(4-toluidino)pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Gillessen, Jutta
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, D-6500, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1985), 29(4), 385-97
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



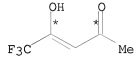
I

AB The title compds. I (R = Me, Et, Me2CH, Me3C, Me2CHCH2CH2) were prepared by cyclization of p-MeC6H4NHC(:NH)NH2 with RCOCH:C(OH)CF3. I exhibited antidiabetic, antimycotic, trichomonocidal and herbicidal activity.

RX(1) OF 5 A + B ===> C

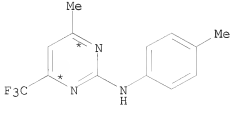


A



B

(1)



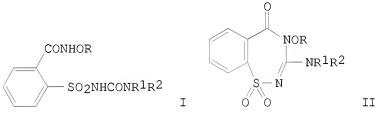
C

RX(1) RCT A 54015-04-2, B 453-33-8
RGT D 497-19-8 Na2CO3
PRO C 104312-45-0

L3 ANSWER 61 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:115087 CASREACT
TITLE: Heterocyclic 1-(2-hydroxyaminocarbonylphenylsulfonyl)urea derivatives
INVENTOR(S): Diehr, Hans Joachim; Fest, Christa; Kirsten, Rolf; Kluth, Joachim; Mueller, Klaus Helmut; Pfister, Theodor; Priesnitz, Uew; Riebel, Hans Joachim; Roy, Wolfgang
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 62 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

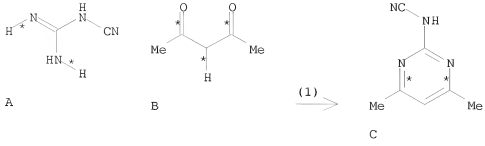
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3516435	A1	19860313	DE 1985-3516435	19850508
EP 173958	A2	19860312	EP 1985-110835	19850819
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4704158	A	19871103	US 1985-769225	19850823
AU 8546656	A	19860306	AU 1985-46656	19850826
DD 238524	A5	19860827	DD 1985-280079	19850828
CA 1223592	A1	19870630	CA 1985-489588	19850828
DK 8503927	A	19860301	DK 1985-3927	19850829
JP 61069761	A	19860410	JP 1985-188713	19850829
ZA 8506594	A	19860430	ZA 1985-6594	19850829
BR 8504158	A	19860624	BR 1985-4158	19850829
HU 39075	A2	19860828	HU 1985-3283	19850829
PRIORITY APPLN. INFO.:			DE 1984-3431927	19840830
			DE 1985-3516435	19850508

GI



AB The title compds. [I; R = (un)substituted alkyl, alkenyl, alkynyl, aryl, aralkyl, cycloalkyl, cycloalkylalkyl; R1 = H, (un)substituted alkyl, alkenyl, alkynyl, aralkyl; R2 = (un)substituted, (un)fused 6-membered aromatic heterocycle containing ≥1 N atom] are prepared as herbicides (no data). Thus, II (R = Me, R1 = H, R2 = 4,6-dimethylpyrimidin-2-yl) (preparation given) was stirred with HCl for 15 h to give the corresponding I.

RX(1) OF 12 A + B ===> C...

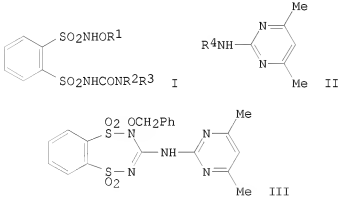


RX(1) RCT A 461-58-5, B 123-54-6
PRO C 55474-90-3

L3 ANSWER 62 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:97492 CASREACT
TITLE: 1-[2-(Alkoxysulfamoyl)phenylsulfonyl]-3-pyrimidinylureas
INVENTOR(S): Diehr, Hans Joachim; Fest, Christa; Kirsten, Rolf; Kluth, Joachim; Mueller, Klaus Helmut; Pfister, Theodor; Priesnitz, Uwe; Riebel, Hans Jochem; Roy, Wolfgang
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3431932	A1	19860306	DE 1984-3431932	19840830
EP 173324	A1	19860305	EP 1985-110838	19850819
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
US 4658027	A	19870414	US 1985-769184	19850823
AU 8546658	A	19860306	AU 1985-46658	19850826
CA 1230338	A1	19871215	CA 1985-489579	19850828
DK 8503930	A	19860301	DK 1985-3930	19850829
JP 61069765	A	19860410	JP 1985-188717	19850829
ZA 8506588	A	19860430	ZA 1985-6588	19850829
BR 8504161	A	19860624	BR 1985-4161	19850829
HU 39429	A2	19860929	HU 1985-3281	19850829
PRIORITY APPLN. INFO.:			DE 1984-3431932	19840830

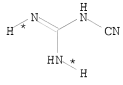
OTHER SOURCE(S): MARPAT 105:97492
GI



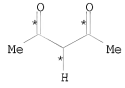
AB The title compds. I [R1 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aralkyl, aryl; R2 = H, (un)substituted alkyl, alkenyl, alkynyl, aralkyl; R3 = (un)substituted heteroaryl] were prepared as herbicides (no data). Thus, H2NC(:NH)NHCN was cyclocondensed with

MeCOCH2COMe to give amino-pyrimidine II (R4 = cyano). This was condensed with PhCH2ONH2 to give II [R4 = C(:NH)NHOCH2Ph]. The latter was cyclocondensed with 1,2-(ClSO2)2C6H4 to give benzodisultam III. III was hydrolyzed with aqueous NaOH to give I (R1 = CH2Ph, R2 = H, R3 = 4,6-dimethyl-2-pyrimidinyl).

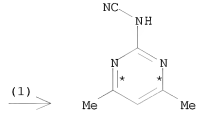
RX(1) OF 12 A + B ===> C...



A



B



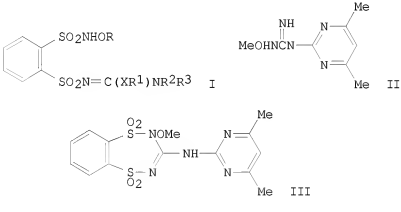
C

RX(1) RCT A 461-58-5, B 123-54-6
PRO C 55474-90-3

L3 ANSWER 63 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:78952 CASREACT
TITLE: Pyrimidinyl- and triazinyl(sulfamoylphenyl)isoureas and -thioureas
INVENTOR(S): Diehr, Hans Joachim; Fest, Christa; Kirsten, Rolf; Kluth, Joachim; Mueller, Klaus Helmut; Pfister, Theodor; Priesnitz, Uwe; Riebel, Hans Jochem; Roy, Wolfgang; et al.
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 59 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3431930	A1	19860306	DE 1984-3431930	19840830
EP 173316	A2	19860305	EP 1985-110827	19850819
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4659364	A	19870421	US 1985-769192	19850823
AU 8546660	A	19860306	AU 1985-46660	19850826
CA 1221697	A1	19870512	CA 1985-489586	19850828
DD 246246	A5	19870603	DD 1985-280074	19850828
DK 8503944	A	19860301	DK 1985-3944	19850829
JP 61060653	A	19860328	JP 1985-188715	19850829
ZA 8506590	A	19860430	ZA 1985-6590	19850829
BR 8504160	A	19860624	BR 1985-4160	19850829
HU 39165	A2	19860828	HU 1985-3282	19850829

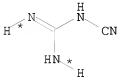
PRIORITY APPLN. INFO.: DE 1984-3431930 19840830
OTHER SOURCE(S): MARPAT 105:78952
GI



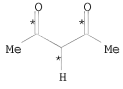
AB The title compds. [I; R = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl; R1 = R, heteroaryl; R2 = H, alkyl, alkenyl, alkynyl, aralkyl; R3 = (un)substituted, N-containing heterocyclyl; X = S, O]

were prepared as herbicides and plant growth regulators (no data). Thus, NCN:C(NH2)2 was cyclocondensed with (MeCO)2CH2 to give 2-(cyanoamino)-4,6-dimethylpyrimidine. This was aminolyzed with H2NOMe to give pyrimidinylguanidine II. The latter was cyclocondensed with 1,2-(ClSO2)2C6H4 to give cyclic benzenedisulfonamide III. This was ring opened with basic MeOH to give I (R = R1 = Me, R2 = H, R3 = 4,6-dimethyl-2-pyrimidinyl, X = O).

RX(1) OF 9 A + B ===> C...

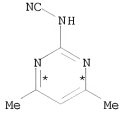


A



B

(1)



C

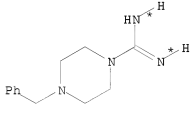
RX(1) RCT A 461-58-5, B 123-54-6
PRO C 55474-90-3

L3 ANSWER 64 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:42844 CASREACT
TITLE: 2-(1-Piperazinyl)pyrimidine derivatives
INVENTOR(S): Yokoyama, Keiichi; Ishida, Tatsuyoshi; Isayama, Shigeru; Kato, Kohji; Kitahara, Takumi; Furuya, Yoshiaki
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

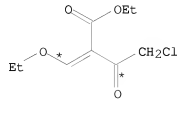
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8601798	A1	19860327	WO 1985-JP500	19850907
W: US				
RW: DE, FR, GB, IT				
JP 61065873	A	19860404	JP 1984-186542	19840907
JP 05022703	B	19930330		
EP 192783	A1	19860903	EP 1985-904492	19850907
EP 192783	B1	19910417		
R: DE, FR, GB, IT				
US 4742165	A	19880503	US 1986-865566	19860502
CA 1288429	C	19910903	CA 1986-508532	19860506
PRIORITY APPLN. INFO.:			JP 1984-186542	19840907
			WO 1985-JP500	19850907

GI For diagram(s), see printed CA Issue.
AB The title compds. [I; R1 = H, aralkyl; Y = oxaalkylene, azaalkylene, oxaazaalkylene, etc.], useful as herbicides, were prepared Thus, piperazine derivative II was condensed with piperidinedione derivative III under reflux to give 69% pyridopyrimidinone IV. 10% Aqueous prepns. of I were effective against most common weeds.

RX(4) OF 81 ...J + F ===> K...

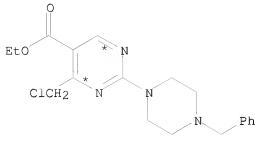


J



F

(4)



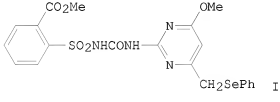
K
YIELD 86%

RX(4) RCT J 7773-69-5, F 91168-75-1
       PRO K 104966-06-5

L3 ANSWER 65 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:6520 CASREACT
TITLE: Herbicidal 1-(2-pyrimidinyl)-3-(phenylsulfonyl)ureas.
INVENTOR(S): Wexler, Barry A.; Zimmerman, William T.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
SOURCE: U.S., 59 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4563211	A	19860107	US 1984-590882	19840319

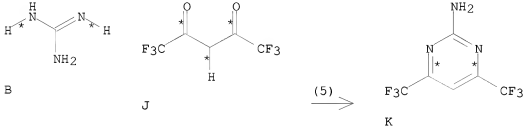
PRIORITY APPLN. INFO.: US 1984-590882 19840319
OTHER SOURCE(S): MARPAT 105:6520
GI



I

AB R1SO2NHCONR2R3 (R1 = alkyl, alkoxy-, sulfamoyl-, halo-, oxadiazolyl-, isoxazolyl-, pyrazolyl-, or furylphenyl, etc.; R2 = H, Me; R3 = substituted 2-pyrimidinyl) were prepared, and they exhibited herbicidal activity. A 2-aminopyrimidine derivative was treated with 2-MeO2CC6H4SO2NCO in CH2Cl2 to give pyrimidinylurea derivative I.

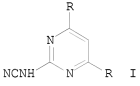
RX(5) OF 13 B + J ===> K...



B J (5) K

RX(5) RCT B 113-00-8, J 1522-22-1
PRO K 102581-66-8

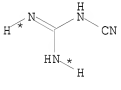
L3 ANSWER 66 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 104:168429 CASREACT
TITLE: Antimycotics. XIX. 4,6-Disubstituted 2-(cyanamino)pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Sellheim, Michael
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, D-6500, Fed. Rep. Ger.
SOURCE: Journal of Heterocyclic Chemistry (1985), 22(3), 721-3
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

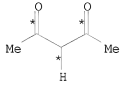


I

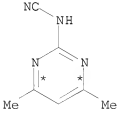
AB The reaction of dicyandiamide, NCNHC(:NH)NH2, with β-diketones HOCR:CHCOR (R = Me, Et, Pr) leads to 2-(cyanoamino)pyrimidines I (same R). I (R = Me) exhibits fungistatic and nematocidal activity.

RX(1) OF 4 A + B ===> C


A


B

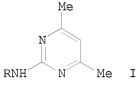
(1)


C

RX(1) RCT A 461-58-5, B 123-54-6
RGT D 141-52-6 NaOEt

PRO C 55474-90-3
SOL 64-17-5 EtOH

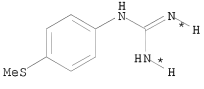
L3 ANSWER 67 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 104:129862 CASREACT
TITLE: Antibacterial drugs. X: 2-(methylthioanilino)pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Tantawy, Atif; Stratmann, Joerg
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, 6500, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1985), 318(11), 1043-5
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



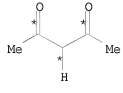
I

AB Title pyrimidines I (R = m- or p-MeSC6H4) were prepared by condensing (methylthiophenyl)guanidines RNHC(NH2):NH with acetylacetone in EtOH. The I were highly active against Aerobacter aerogenes and against the fungus Plasmopara viticola.

RX(1) OF 2 A + B ===> C

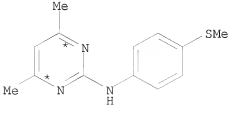


A



B

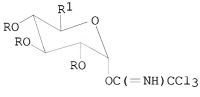
(1)



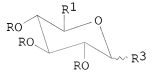
C

RX(1) RCT A 71198-45-3, B 123-54-6
       PRO C 100936-27-4
       SOL 64-17-5 EtOH

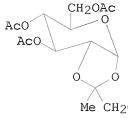
L3 ANSWER 68 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 104:51038 CASREACT
TITLE: O-Glycosyl imidates. 19. Reaction of glycosyl trichloroacetimidates with silylated C-nucleophiles
AUTHOR(S): Hoffmann, Michael G.; Schmidt, Richard R.
CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1985), (12), 2403-19
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I



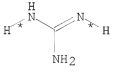
II



III

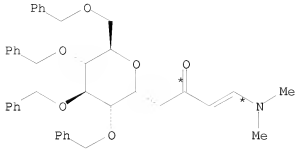
AB Reaction of the trichloroacetimidates I (R = CH2Ph, R1 = CH2OR, H) with Me3SiOCR2:CH2 [R2 = Ph, CMe3, Me, CH2CH2CH:CH2, (CH2)4OCH2Ph] or CH2:CHCH2SiMe3 as C-nucleophiles yields with ZnCl2 as catalyst mainly or exclusively α-C-glycosides II (R3 = CH2COR2, alkyl). The reactions with Me3SiCN to form α-C-glycosyl cyanides II (R3 = cyano) were carried out in the presence of Me3SiO3SCF3 as catalyst. Silyl enol ethers reacted with I (R = Ac, R1 = CH2OAc) to give 1,3-dicarbonyl derivs. III. Reaction of II (R = CH2Ph, R1 = CH2OCH2Ph, R3 = CH2COPh) with Me3COCH(NMe2)2 and subsequently with N2H4, acetamidine, or guanidine gives preferentially β-C-nucleosides. However, α-homo-C-nucleosides are obtained from the corresponding reactions with other II.

RX(36) OF 120 ...BY + CB ===> CG



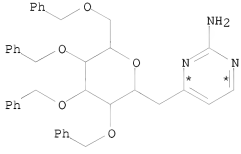
BY: CM 1

BY: CM 2



CB

(36)



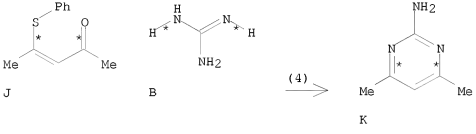
CG

RX(36) RCT BY 594-14-9, CB 99701-91-4
RGT S 141-52-6 NaOEt
PRO CG 99701-93-6
SOL 64-17-5 EtOH

L3 ANSWER 69 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 104:50839 CASREACT
TITLE: Reactions of β-sulfenyl α,β-unsaturated ketones with guanidine, amidines, and diamines
AUTHOR(S): Nishio, Takehiko; Tokunaga, Tatsuhiro; Omote, Yoshimori
CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan
SOURCE: Journal of Heterocyclic Chemistry (1985), 22(2), 405-7
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cyclocondensation of RCOCH:CR1SR2 (I, R = Ph, R1 = Me, R2 = Et; R = R1 = Me, R2 = Ph; R = R1 = Ph, R2 = Et) with R3C(:NH)NH2 (R3 = NH2, Me, Ph) gave pyrimidine derivs. in 14-76% yields. Cyclocondensation of I with ethylenediamine or o-(H2N)2C6H4 afforded 1,4-diazepines.

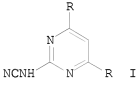
RX(4) OF 14 J + B ===> K



J B K

RX(4) RCT J 70769-79-8, B 113-00-8
RGT D 1310-73-2 NaOH
PRO K 767-15-7
SOL 64-17-5 EtOH

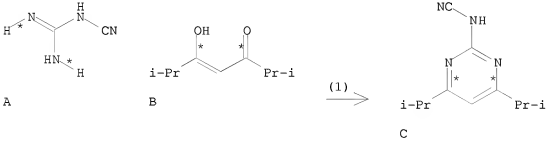
L3 ANSWER 70 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 103:215254 CASREACT
TITLE: Trichomonacidal agents. 2. Branched chain 4,6-disubstituted 2-(cyanoamino)pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Sellheim, Michael
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, 6500, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1985), 318(9), 801-6
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

AB The reaction of dicyandiamide with (RCO)2CH2 (R = CHMe2, CMe3) yields the 2-(cyanoamino)pyrimidines I. Spectroscopic evidence, particularly from 1H- and 13C-NMR data, shows that the tautomeric 2-(cyanoamino)- and 2-(cyanoimino)pyrimidine forms exist in equilibrium I (R = CMe3) exhibits trichomonacidal, antiviral, antimycotic, and antidiabetic activities.

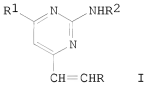
RX(1) OF 2 A + B ===> C



A B C

RX(1) RCT A 461-58-5, B 34136-02-2
RGT D 124-41-4 NaOMe
PRO C 99225-23-7
SOL 64-17-5 EtOH

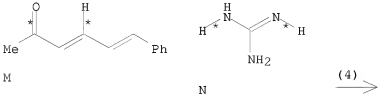
L3 ANSWER 71 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 103:178216 CASREACT
TITLE: Heterocycles. 80. Reactions of guanidine and thiourea with α,β,γ,δ-unsaturated ketones
AUTHOR(S): Wendelin, Winfried; Schramm, Hans Wolfgang; Blasi-Rabassa, Andreas
CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Graz, Graz, A-8010, Austria
SOURCE: Monatshefte fuer Chemie (1985), 116(3), 385-400
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



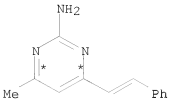
I

AB Guanidine and phenylguanidine react with R(CH:CH)2COR1 (R = Ph, R1 = Me, Ph, substituted Ph, 4-pyridyl; R = 2-ClC6H4, R1 = 4-ClC6H4) to give 6-styryl-2-pyrimidinamines I (R1 = H, Ph). Efforts to stabilize the intermediate dihydropyrimidines by introduction of electron-withdrawing substituents were not successful. Similarly, thiourea reacts with Ph(CH:CH)2COPh to afford 4-phenyl-6-phenethylpyrimidinethione. Action of guanidine on 1,3,5-triphenylpentadienone and on the 5-(3-chlorophenyl) analog (II) yields 4,6-diphenyl- and 4-(3-chlorophenyl)-6-phenyl-2-pyrimidinamine, resp. However, heating thiourea with II in NaOBu-BuOH gives the expected 4,6-diphenyl-4-styryldihydropyrimidinethione. Treating thiourea with triphenylpentadienone gave 2-(4,6-diphenyl-2-thioxohexahydro-4-pyrimidinyl)acetophenone, whose conformation was deduced by NMR.

RX(4) OF 27 M + N ===> O



M N

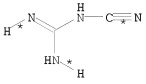


O

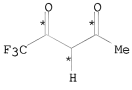
RX(4) RCT M 4173-44-8, N 113-00-8
PRO O 98928-85-9
SOL 71-43-2 Benzene

L3 ANSWER 72 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 103:87833 CASREACT
TITLE: Antineoplastics. XVI.
4-Alkyl-6-(trifluoromethyl)-2-ureidopyrimidines
AUTHOR(S): Kreutzberger, Alfred; Sellheim, Michael
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, D-6500, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1985), 27(2), 203-12
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
AB The reaction of NCNHC(:NH)NH2 with trifluoromethyl-substituted β-diketones gives 4-alkyl-6-trifluoromethyl-2-ureidopyrimidines. Thus, 4-methyl-6-trifluoromethyl-2-ureidopyrimidine is formed from 1,1,1-trifluoro-2,4-pentanedione, and 4-ethyl-6-trifluoromethyl-2-ureidopyrimidine from 1,1,1-trifluoro-2,4-hexanedione.

RX(1) OF 3 A + B ===> C

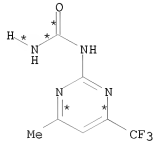


A



B

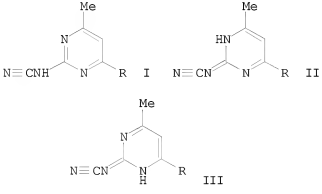
(1)



C

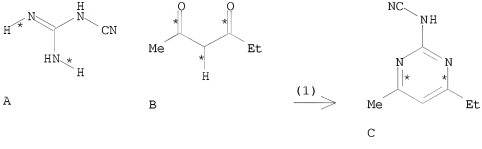
RX(1) RCT A 461-58-5, B 367-57-7
RGT D 1310-73-2 NaOH
PRO C 75945-77-6
SOL 64-17-5 EtOH, 7732-18-5 Water

L3 ANSWER 73 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 103:54030 CASREACT
TITLE: Herbicides, III. Synthesis of 4,6-dialkyl-2-(cyanoamino)pyrimidines and studies of their structures by carbon-13 NMR spectroscopy
AUTHOR(S): Kreutzberger, Alfred; Sellheim, Michael
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, 6500, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1985), 318(5), 385-92
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



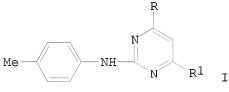
AB Unsym. substituted pyrimidines I (R = Et, Bu, pentyl) were prepared in 3-22% yield by cyclocondensation of dicyandiamide with MeCOCH2COR. I are in equilibrium with (cyanoimino)pyrimidines II and III according to 13C NMR. The known 2-(cyanoamino)-4,6-diethylpyrimidine has herbicidal activity.

RX(1) OF 4 A + B ===> C



RX(1) RCT A 461-58-5, B 3002-24-2
RGT D 141-52-6 NaOEt
PRO C 97323-41-6
SOL 64-17-5 EtOH

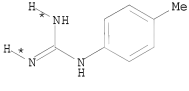
L3 ANSWER 74 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 103:22549 CASREACT
TITLE: Antimycotic agents, XVIII. Aromatically substituted 2-(4-toluidino)pyrimidines
AUTHOR(S): Keutzberger, Alfred; Gillessen, Jutta
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, 6500, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1985), 318(4), 370-4
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



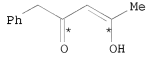
I

AB Pyrimidines I (R = Me, R1 = Ph, CH2Ph, 2-furyl; R = R1 = Ph) were obtained in 30-50% yield by fusing 4-MeC6H4NHC(:NH)NH2 with RCOCH2COR1 and Na2CO3.

RX(2) OF 4 A + E ===> F



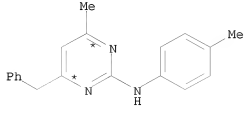
A



E

(2)

F: CM 1

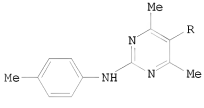


F: CM 2

RX(2) RCT A 54015-04-2, E 96924-36-6
RGT D 497-19-8 Na2CO3

PRO F 96924-40-2

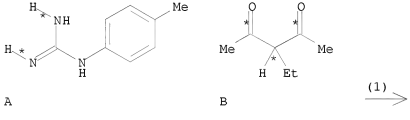
L3 ANSWER 75 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 102:185044 CASREACT
TITLE: Antidiabetic hormones. III. 4,5,6-Trisubstituted 2-(4-toluidino)pyrimidine
AUTHOR(S): Kreutzberger, Alfred; Gillessen, Jutta
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ. Mainz, Mainz, Fed. Rep. Ger.
SOURCE: Journal of Heterocyclic Chemistry (1984), 21(6), 1639-40
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



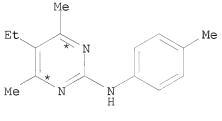
I

AB 2,4-Pentanediones MeCOCHRCOMe (R = Me, Et) were cyclocondensed with 4-MeC6H4NHC(:NH)NH2 to give toluidinopyrimidines I.

RX(1) OF 1 A + B ===> C



A B (1)



C
YIELD 16%

RX(1) RCT A 54015-04-2, B 1540-34-7

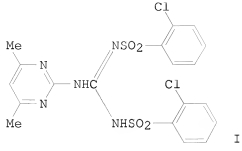
PRO C 96238-98-1

L3 ANSWER 76 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 102:95661 CASREACT
TITLE: Guanidine derivatives
INVENTOR(S): Moriya, Koichi; Pfister, Theodor; Riebel, Jochem; Eue, Ludwig; Schmidt, Robert R.; Luerssen, Klaus
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 134 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3334455	A1	19840906	DE 1983-3334455	19830923
AU 8424259	A	19840906	AU 1984-24259	19840208
AU 561585	B2	19870514		
US 4602938	A	19860729	US 1984-578345	19840209
EP 121082	A1	19841010	EP 1984-101910	19840223
EP 121082	B1	19891108		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 47845	T	19891115	AT 1984-101910	19840223
BR 8400887	A	19841009	BR 1984-887	19840227
DK 8401484	A	19840905	DK 1984-1484	19840229
JP 59167570	A	19840921	JP 1984-37415	19840301
DD 223055	A5	19850605	DD 1984-260469	19840301
DD 229691	A5	19851113	DD 1984-277164	19840301
IL 71118	A	19870916	IL 1984-71118	19840301
HU 34324	A2	19850328	HU 1984-854	19840302
HU 198611	B	19891128		
ZA 8401585	A	19850626	ZA 1984-1585	19840302
CA 1233180	A1	19880223	CA 1984-448787	19840302
US 4721785	A	19880126	US 1986-853822	19860418
US 4725305	A	19880216	US 1986-931368	19861114
US 4725303	A	19880216	US 1986-931380	19861114
US 4797484	A	19890110	US 1987-5800	19870116
US 4743294	A	19880510	US 1987-41260	19870422
US 4880932	A	19891114	US 1987-44083	19870429
US 4844730	A	19890704	US 1988-224973	19880727

PRIORITY APPLN. INFO.:
DE 1983-3307679 19830304
DE 1983-3334455 19830923
US 1984-578345 19840209
EP 1984-101910 19840223
DE 1984-3431924 19840830
DE 1984-3431925 19840830
DE 1985-3517821 19850517
DE 1985-3517842 19850517
US 1985-769222 19850823
US 1985-769271 19850823
US 1986-853822 19860418
US 1987-44083 19870429

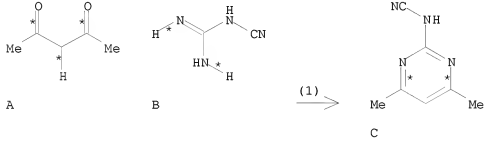
GI



I

AB Herbicidal plant growth inhibiting (no data) RR1NC(:NR2)NHR3 [R = H, R4S(O)n, (un)substituted alkyl, cycloalkyl, alkenyl, alkynyl; R1 = H, OH, Me3Si, R4S(O)n, (un)substituted alkyl, cycloalkyl, alkenyl, alkynyl, aryl, heterocyclyl, amino; RR1N = heterocyclyl; R2 = H, R4S(O)n; R3 = halo, cyano, HCO, (un)substituted alkyl, alkoxy, heterocyclyl, amino; R4 = (un)substituted alkyl, aryl, heteroaryl; n = 0-2] and their tautomers and salts were prepared Thus, 4,6-dimethylpyrimidine was condensed with Na2NCN to give 2-(cyanoamino)-4,6-dimethylpyrimidine. This was treated with MeONH2.HCl to give N-(4,6-dimethyl-2-pyrimidinyl)-N'-methoxyguanidine. This was acylated with 2-ClC6H4SO2Cl to give diacylated guanidine I.

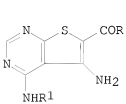
RX(1) OF 19 A + B ===> C...



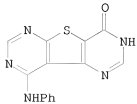
A B C

RX(1) RCT A 123-54-6, B 461-58-5
PRO C 55474-90-3

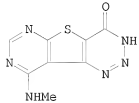
L3 ANSWER 77 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 102:62175 CASREACT
TITLE: Heterocyclic studies. Part 43. Thieno[2,3-d:4,5-d']dipyrimidines
AUTHOR(S): Clark, Jim; Hitiris, George
CORPORATE SOURCE: Dep. Chem. Appl. Chem., Univ. Salford, Salford, M5 4WT, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (9), 2005-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



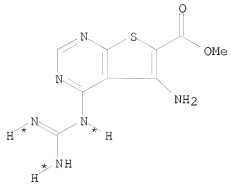
II



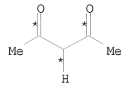
III

AB Reaction of 5-aminothieno[2,3-d]pyrimidine-6-carboxamides or -6-carboxylic esters with a variety of reagents, e.g., HC(OEt)3, (H2N)2CO, gave thieno[2,3-d:4,5-d']dipyrimidines. E.g., reaction of thienopyrimidine I (R = OMe, R1 = Ph) with HCONH2 at 160° for 4 h gave 76% thienodipyrimidine II. Reaction of I (R = NH2, R1 = Me) with HNO2 gave 79% III, the first pyrimido[5',4':4,5]thieno[3,2-d]-1,2,3-triazine.

RX(19) OF 37 ...AJ + AK ===> AL...

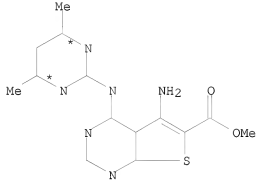


AJ



AK

(19)



AL
YIELD 74%

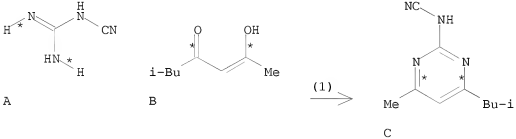
RX(19) RCT AJ 94556-67-9, AK 123-54-6
PRO AL 94556-72-6

L3 ANSWER 78 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 102:24572 CASREACT
TITLE: Antiviral agents, XXVI. Synthesis of 4,6-disubstituted 2-(cyanoamino)pyrimidines and studies of their structure by mass spectroscopy
AUTHOR(S): Kreutzberger, Alfred; Sellheim, Michael
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ. Mainz, Mainz, Fed. Rep. Ger.
SOURCE: Chemiker-Zeitung (1984), 108(7-8), 253-5
CODEN: CMKZAT; ISSN: 0009-2894
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

I

AB NCNHC(:NH)NH2 was condensed with HOCMe:CHCOCH2CHMe2 in 10% aqueous K2CO3 for 5 days at room temperature to give (cyanoamino)pyrimidine I (R = CHMe2). The radical •NHCN and the neutral particle (CN)2 are formed as characteristic fragments during the mass spectrometric degradation of (cyanoamino)pyrimidines, e.g., I (R = H). The formation of a pyrazole radical ion, which occupies a key position during degradation of analogous pyrimidines, occurs during loss of the significant fragments •NHCN and (CN)2.

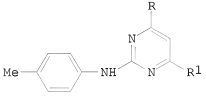
RX(1) OF 1 A + B ===> C



A B C

RX(1) RCT A 461-58-5, B 81100-84-7
PRO C 93958-92-0
CAT 584-08-7 K2CO3, 298-14-6 KHCO3

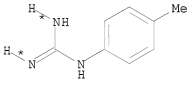
L3 ANSWER 79 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 101:211094 CASREACT
TITLE: Antidiabetic agents, II. 2-(4-Toluidino)pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Gillessen, Jutta
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ. Mainz, Mainz, 6500, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1984), 317(9), 749-53
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



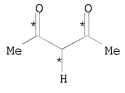
I

AB Condensations of 4-tolylguanidine with RCOCH2COR1 (R = R1 = Me, Et, Pr, CHMe2, CMe3; R = Me, R1 = Et, CH2CHMe2) yield the 2-(4-toluidino)pyrimidines I which comprise compds. with antidiabetic and antimycotic activities. Thus I (R = R1 = Me) at 50 mg/kg orally in guinea pigs lowered blood sugar levels by 12%.

RX(1) OF 7 A + B ===> C

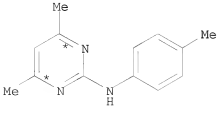


A



B

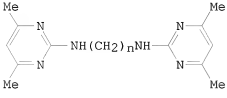
(1)



C
YIELD 80%

RX(1) RCT A 54015-04-2, B 123-54-6
PRO C 81261-68-9

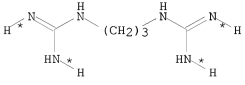
L3 ANSWER 80 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 101:191823 CASREACT
TITLE: Methods for obtaining bisaminopyrimidines bridged by a polymethylene chain
AUTHOR(S): Menichi, Gabriel; Hubert-Habart, Michel
CORPORATE SOURCE: Sect. Phys. Chim., Inst. Curie, Paris, 75231, Fr.
SOURCE: Journal of Heterocyclic Chemistry (1984), 21(1), 209-13
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



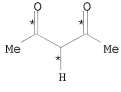
I

AB N(2),N'(2')-αω-Alkandiylbis(2-aminopyrimidines) e.g. I (n = 3, 4, 6, 8) are the sole products obtained by condensation of several polymethylene bisguanidines on Et ethoxymethylenemalonate, 3-methylchromone, flavone, acetylacetone, acetylacetaldehyde dimethylacetal and 3-acetyl-2-ethylbenzofuran.

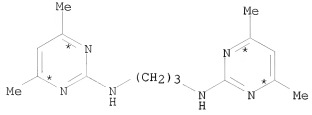
RX(16) OF 37 ...E + 2 X ===> Y



●2 HBr



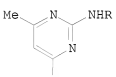
E 2 X (16)

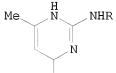


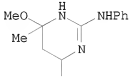
Y
YIELD 75%

RX(16) RCT E 52780-73-1, X 123-54-6
        PRO Y 92736-21-5

L3 ANSWER 81 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 101:191821 CASREACT
TITLE: Dihydropyrimidines and related structures. I. N2-Substituted 2-pyrimidinamines and dihydro-2-pyrimidinamines by reaction of phenylbutenones and monosubstituted guanidines
AUTHOR(S): Wendelin, Winfried; Schermanz, Karl
CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Graz, Graz, A-8010, Austria
SOURCE: Journal of Heterocyclic Chemistry (1984), 21(1), 65-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

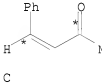

I

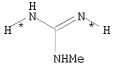

II


III

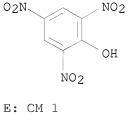
AB H2NC(:NH)NHR (R = Me, PhCH2) reacted with PhCH:CHCOMe and H2NC(:NH)NHCH2Ph with PhCOCH:CHMe under atmospheric O to give pyrimidine I (R = Me, PhCH2). Dihydropyrimidines II, probable intermediates in the reaction, could not be isolated. Heating H2NC(:NH)NHRCR (R = Ph, p-MeOC6H4) with PhCH:CHCOMe gave II. II (R = Ph) reacted with MeOH to give pyrimidinamine III. I (R = Ph) was heated to give I (R = Ph). The low stability of II is attributed to their strong basicity.

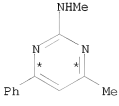
RX(2) OF 12 C + D ===> E


C


D

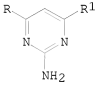
(2)

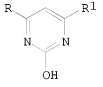

E: CM 1
YIELD 21%


E: CM 2
YIELD 21%

RX(2) RCT C 122-57-6, D 471-29-4
PRO E 89242-68-2

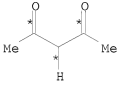
L3 ANSWER 82 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 101:171201 CASREACT
TITLE: A novel reaction of cyanamide with 1,3-diketones
AUTHOR(S): Miller, Audrey
CORPORATE SOURCE: Dep. Chem., Univ. Connecticut, Storrs, CT, 06268, USA
SOURCE: Journal of Organic Chemistry (1984), 49(21), 4072-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

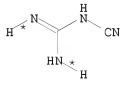

I


II

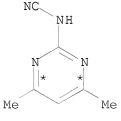
AB Pyrimidines I and II (R = Me, CF3; R1 = Me, CHMe2, Ph) were obtained from RCOCH2COR1. Thus, MeCOCH2COMe was treated with H2NCN to give I (R = R1 = Me), II (R = R1 = Me), MeC(NH2):CHCOMe, MeC(:NCONH2)CH:C(OH)Me, and MeC(:NCN)CH:C(OH)Me.

RX(6) OF 26 E + K ===> L


E

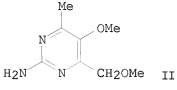

K

(6)


L

RX(6) RCT E 123-54-6, K 461-58-5
PRO L 55474-90-3

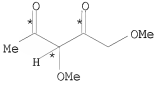
L3 ANSWER 83 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 101:55042 CASREACT
TITLE: 5-Hydroxypyrimidines. V. Condensation of 1,3-dimethoxyacetylacetone with guanidine and thiourea
AUTHOR(S): Wang, Shiyu; Zhang, Pang
CORPORATE SOURCE: Dep. Chem., Peking Univ., Beijing, Peop. Rep. China
SOURCE: Youji Huaxue (1984), (2), 111-13
CODEN: YCHHDX; ISSN: 0253-2786
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



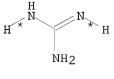
II

AB Heating a mixture of 0.047 mol MeCOCH(OMe)COCH2OMe (I) with 0.042 mol guanidine carbonate at 30-40° and then 60° gave 28.3% pyrimidine derivative II. I did not react with urea or thiourea. Reaction of 4 g I with 3.5 g MeSC(:NH)NH2 (III) in the presence of NaOMe gave 0.8 g MeOCH2CMe:NC(:NH)SMe.MeOCH2CO2H and 0.2 g III.MeOCH2CO2H.

RX(1) OF 2 A + B ===> C



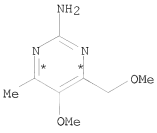
A



B: CM 1

B: CM 2

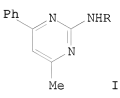
(1)



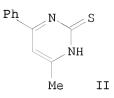
C
YIELD 28%

RX(1) RCT A 85061-10-5, B 124-46-9
PRO C 91044-63-2

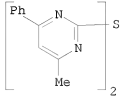
L3 ANSWER 84 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 100:121009 CASREACT
TITLE: Heterocycles. 76. Reactions of monosubstituted guanidines with 1-phenyl-1,3-butanedione
AUTHOR(S): Wendelin, Winfried; Schermanz, Karl; Schweiger, Klaus; Fuchsgruber, Alfred
CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Graz, Graz, A-8010, Austria
SOURCE: Monatshefte fuer Chemie (1983), 114(12), 1371-9
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I



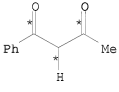
II



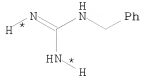
III

AB H2NC(:NH)NHR (R = Me, CH2Ph, Ph) react with PhCOCH2COMe to yield exclusively pyrimidinamines I. The formation of pyrimidinimines was observed The structure of I (R = Ph) was determined by comparison with an authentic sample prepared from the pyrimidinthione II via the methylthiopyrimidine. Boiling II with PhNH2-BuOH yields the thiodipyrimidine III.

RX(1) OF 4 A + B ===> C



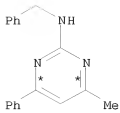
A



● HCl

B

(1)



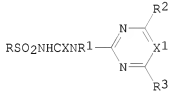
C

RX(1) RCT A 93-91-4, B 1197-49-5
PRO C 89242-69-3
CAT 141-52-6 NaOEt

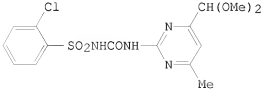
L3 ANSWER 85 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 99:175810 CASREACT
TITLE: Herbicidal sulfonamides
INVENTOR(S): Shapiro, Rafael
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co. , USA
SOURCE: Brit. UK Pat. Appl., 105 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2110692	A	19830622	GB 1982-34702	19821206
GB 2110692	B	19850717		
DK 8205365	A	19830608	DK 1982-5365	19821202
CA 1221698	A1	19870512	CA 1982-416863	19821202
BR 8207018	A	19831011	BR 1982-7018	19821203
AU 8291151	A	19830616	AU 1982-91151	19821206
AU 553872	B2	19860731		
EP 84224	A1	19830727	EP 1982-306492	19821206
EP 84224	B1	19861008		
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
HU 30867	A2	19840428	HU 1982-3907	19821206
ZA 8208949	A	19840725	ZA 1982-8949	19821206
IL 67423	A	19860930	IL 1982-67423	19821206
AT 22684	T	19861015	AT 1982-306492	19821206
JP 58116472	A	19830711	JP 1982-213490	19821207
US 4629494	A	19861216	US 1985-723450	19850415
US 4655823	A	19870407	US 1985-734331	19850515
US 4806142	A	19890221	US 1986-896091	19860813
PRIORITY APPLN. INFO.:			US 1981-328018	19811207
			US 1982-434038	19821020
			EP 1982-306492	19821206
			US 1983-543835	19831020
			US 1985-723450	19850415

OTHER SOURCE(S): MARPAT 99:175810
GI



I

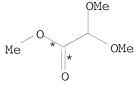


II

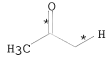
AB Sulfonylureas I [R = substituted aryl, heteroaryl, aryloxy, benzyl; R1 = H, Me; R2 = Me, OMe, Cl, Et, OEt; R3 = (un)substituted CH2OH, CH2SH, CHO, alkoxy; X = O, S; X1 = CH, N] were prepared Thus, (MeO)2CHCO2Me was treated with acetone to give (MeO)2CHCOCH2COMe which was treated with guanidine carbonate to give 2-amino-4-dimethoxymethyl-6-methylpyrimidine. Treatment of this amine with 2-ClC6H4SO2NCO gave II which had herbicidal activity against various weeds at 0.05 kg/ha post-emergence.

RX(2) OF 9 D + E + F ===> A

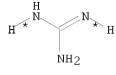
...



D

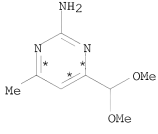


E



F

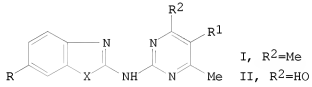
(2)



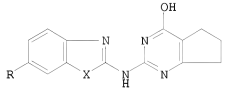
A

RX(2) RCT D 89-91-8, E 67-64-1, F 113-00-8
PRO A 87643-77-4

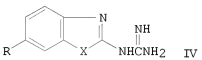
L3 ANSWER 86 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 99:53691 CASREACT
TITLE: Synthesis and mass spectra of some substituted 2-(2'-benzazolylamino)pyrimidines
AUTHOR(S): Singh, S. P.; Prakash, Indra; Tomer, R. K.; Prakash, O. M.; Sawhney, S. N.
CORPORATE SOURCE: Chem. Dep., Kurukshetra Univ., Kurukshetra, 132 119, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(1), 37-42
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I, R^2=Me II, R^2=HO



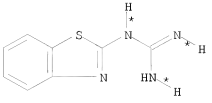
III



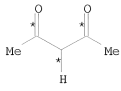
IV

AB The title compds. I and II (R = H, Me, MeO, Cl; R1 = H, Me, Et, CH2CO2Et; X = S, NH, O) and III (R = H, Me, MeO, Cl; X = S, NH, O) were prepared by cyclization of the guanidine IV with MeCOCHR1COMe, MeCOCHR1CO2Et, and Et 2-oxo-2-cyclohexanecarboxylate, resp. Mass spectra studies reveal that there is an initial fragmentation of pyrimidine ring in I via two competitive processes involving either the loss of Me cyanide followed by Me group or vice versa. This mode of fragmentation, however, is completely suppressed in the presence of a methoxyl substituent in the benzothiazole ring which triggers an alternative low-energy pathway. No loss of Me cyanide or Me group has been observed in the mass spectra of II, rather than pyrimidine ring undergoes fission resulting in the initial loss of formyl radical. Several of these compds. exhibit significant antiinflammatory activity.

RX(5) OF 71 K + L ===> M

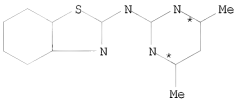


K



L

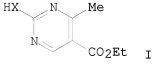
(5)



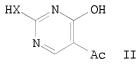
M
YIELD 82%

RX(5) RCT K 2582-07-2, L 123-54-6
PRO M 19604-14-9

L3 ANSWER 87 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 98:72051 CASREACT
TITLE: Recyclization of 5-carbethoxy-4-methyl-2-mercapto(amino, hydroxy)pyrimidines to 5-acetyl-2-mercapto(amino, hydroxy)-4-hydroxypyrimidines
AUTHOR(S): Vartanyan, R. S.; Kazaryan, Zh. V.; Vartanyan, S. A.
CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1982), (11), 1558-9
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



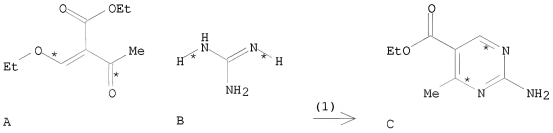
I



II

AB Cyclocondensation of MeCOC(:CHOEt)CO2Et with H2NC(:NH)NH2.HCl or thiourea gave 82 and 76% I (X = NH, S), resp., which when treated with a strong base (NaOEt) recyclize to give 79 and 87% II (X as above). Addnl. obtained was 82% I (X = O).

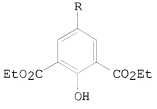
RX(1) OF 9 A + B ===> C...



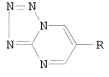
A B C

RX(1) RCT A 3788-94-1, B 113-00-8
PRO C 81633-29-6
CAT 141-52-6 NaOEt

L3 ANSWER 88 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 98:71534 CASREACT
TITLE: Syntheses with aliphatic dialdehydes. XXXV. Syntheses with 1- and 2-adamantylmalonaldehyde
AUTHOR(S): Reichardt, Christian; Wuerthwein, Ernst Ulrich
CORPORATE SOURCE: Fachber. Chem., Univ. Marburg, Marburg, D-3550, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1982), 37B(9), 1187-95
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



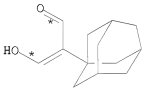
I



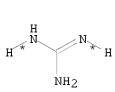
II

AB The reaction of 1- and 2-adamantyl malonaldehyde with suitable electrophiles and nucleophiles yields adamantyl-substituted open-chain e.g. PhNHCH:CRCHO (R = 1- and 2-adamantyl) as well as heterocyclic compds., e.g. II (R = 2-adamantyl), with peculiar properties due to the presence of the lipophilic adamantyl group. The tetrazolo[1,5-a]pyrimidine II (R = 2-adamantyl) exhibits a solvent-dependent tetrazolo-azido valence isomerization reaction.

RX(6) OF 14 E + P ===> Q

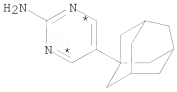


E



P

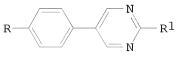
(6)

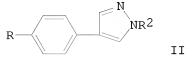


Q
YIELD 74%

RX(6) RCT E 344777-55-5, P 113-00-8
PRO Q 84396-69-0

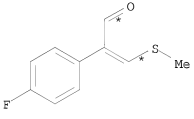
L3 ANSWER 89 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 97:162920 CASREACT
TITLE: A new and facile synthesis of 5-arylpyrimidines and 4-arylpyrazoles
AUTHOR(S): Kano, Shinzo; Yuasa, Yoko; Shibuya, Shiroshi; Hibino, Satoshi
CORPORATE SOURCE: Tokyo Coll. Pharm., Tokyo, 192-03, Japan
SOURCE: Heterocycles (1982), 19(6), 1079-82
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

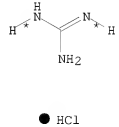

I


II

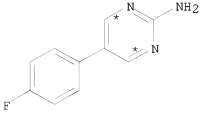
AB The cyclocondensation reaction of acroleins 4-RC6H4C(CHO):CHSMe (R = Me, OMe, F, Cl, CO2Et) with R1C(:NH)NH2 (R1 = H, Me, NH2) and R2NHNH2 (R2 = Me, Ph) gave the resp. pyrimidines I and pyrazoles II; I are useful as antiinflammatory agents (no data). Thus, a mixture of 4-MeC6H4C(CHO):CHSMe, HC(:NH)NH2·HOAc, and Na2CO3 in EtOH was refluxed to give I (R = Me, R1 = H).

RX(19) OF 68 ...D + AE ===> AF


D


AE

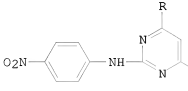
(19)


AF

YIELD 75%

RX(19) RCT D 82525-14-2, AE 50-01-1
PRO AF 31408-40-9

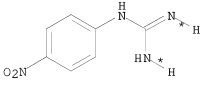
L3 ANSWER 90 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 97:55763 CASREACT
TITLE: Antiviral agents. XXI. Perfluoroalkyl-2-(4-nitroanilino)pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Richter, Barbara
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, 6500, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1982), 20(2), 227-40
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



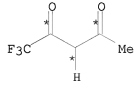
I

AB (Nitroanilino)pyrimidines I (R = CF3, R1 = CF3, Me, Et, CHMe2, CH2CH2CHMe2, CMe3, Ph, 2-naphthyl; R = CF2CF2CF3, R1 = CMe3) were prepared by fusion of 4-O2NC6H4NHC(:NH)NH2 with RCOCH2COR1 in the presence of K2CO3. Mass spectroscopic and IR measurements on the substituted pyrimidines are reported. I (R = R1 = CF3) gave 68% inhibition of Newcastle disease virus at 20 μg/mL.

RX(1) OF 8 A + B ===> C

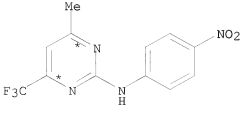


A



B

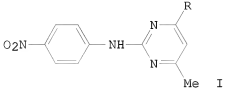
(1)



C

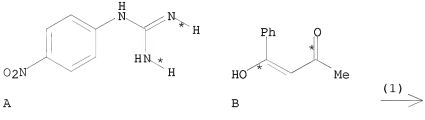
RX(1) RCT A 5901-56-4, B 367-57-7
       PRO C 82501-38-0
       CAT 584-08-7 K2CO3

L3 ANSWER 91 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 95:169117 CASREACT
TITLE: Insecticidal agents. I. Cyclization reactions with 4-nitrophenylguanidine
AUTHOR(S): Kreutzberger, Alfred; Richter, Barbara
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, D-6500, Fed. Rep. Ger.
SOURCE: Chemiker-Zeitung (1981), 105(7-8), 229-32
CODEN: CMKZAT; ISSN: 0009-2894
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

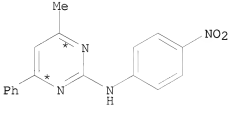


AB Pyrimidines I (R = Ph, CH2Ph, CH2CH2Ph, 2-pyridyl) were obtained in 18.8-38.9% yield by treating 4-O2NC6H4NHC(:NH)NH2 with RCOCH2COMe.

RX(1) OF 4 A + B ===> C



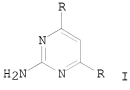
A B (1)



C
YIELD 27%

RX(1) RCT A 5901-56-4, B 1704-14-9
PRO C 79530-01-1

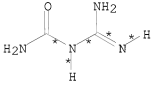
L3 ANSWER 92 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 95:80880 CASREACT
TITLE: 4,6-Dialkylated pyrimidine derivatives
AUTHOR(S): Kreutzberger, Alfred; Schimmelpfennig, Horst
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ. Mainz, Mainz, 6500, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1981), 314(5), 391-4
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



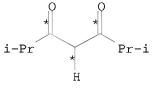
I

AB Refluxing HOCR:CHCOR (R = CHMe2, CMe3) with H2NCONHC(:NH)NH2 in 80% EtOH gave the corresponding aminopyrimidines I (R = CHMe2, CMe3) in 22 or 6% yield, resp., as potential hypnotics.

RX(1) OF 2 A + B ===> C

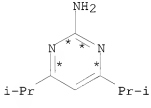


A



B

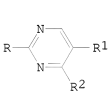
(1)

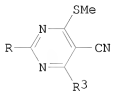


C
YIELD 22%

RX(1) RCT A 141-83-3, B 18362-64-6
PRO C 78641-12-0

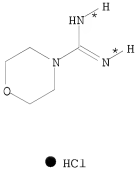
L3 ANSWER 93 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 95:43026 CASREACT
TITLE: Morpholinopyrimidines
AUTHOR(S): Kristen, Helmut; Raddatz, Marianne
CORPORATE SOURCE: Sekt. Chem., Wilhelm-Pieck-Univ. Rostock, Rostock, DDR-2500, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1981), 21(3), 101
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

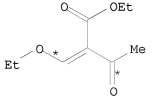

II


III

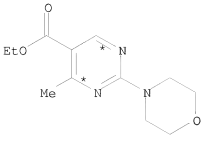
AB Reaction of RC(NH2):NH (I, R = morpholino throughout) with EtOCH:CR1R2 (R1 = R2 = CN; R1 = CO2Et, R2 = CN, COMe, CO2Et) gave 52-88% II (R1 = CN, R2 = NH2; R1 = CO2Et, R2 = NH2, Me, OH, resp.). Reaction of I with (MeS)2C:C(CN)R3 (R3 = CN, CO2Et) gave 43 and 32% III (R3 = NH2, OH, resp.).

RX(3) OF 6 A + F ===> G


A


F

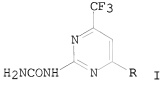
(3)



G
YIELD 74%

RX(3) RCT A 5638-78-8, F 3788-94-1
PRO G 78318-44-2

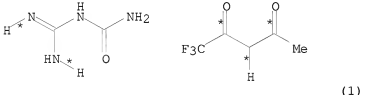
L3 ANSWER 94 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 94:47266 CASREACT
TITLE: Antiviral agents. XVI. Trifluoromethyl-2-ureidopyrimidines
AUTHOR(S): Kreutzberger, Alfred; Schimmelpfennig, Horst
CORPORATE SOURCE: Inst. Pharm., Freie Univ. Berlin, Berlin, D-1000, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1980), 15(6), 511-17
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



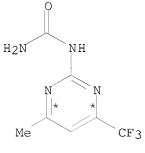
I

AB Trifluoromethyl-2-ureidopyrimidines I (R = Me, Et, Me2CH, Me2CHCH2, Me3C, Me2CHCH2CH2) were prepared by the cyclocondensation of H2NCONHC(:NH)NH2 with the appropriate fluorinated β-diketone.

RX(1) OF 6 A + B ===> C



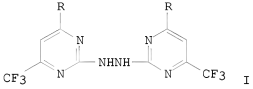
A B (1)



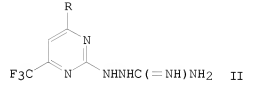
C
YIELD 44%

RX(1) RCT A 141-83-3, B 367-57-7
PRO C 75945-77-6

L3 ANSWER 95 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 91:211363 CASREACT
TITLE: Condensations with hydrazine-N,N'-dicarboxamidine. XXIII. Fluorinated β-diketones as reaction partners
AUTHOR(S): Kreutzberger, Alfred; Risse, Gisa
CORPORATE SOURCE: Inst. Pharm., Freie Univ. Berlin, Berlin, D-1000/33, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1979), 14(2), 131-8
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



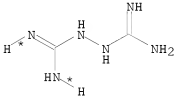
I



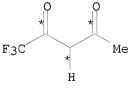
II

AB Condensation of [H2NC(:NH)NH]2 with CF3COCH2COR (R = Me,Et) in the presence of 30% aqueous K2CO3 leads to the pyrimidines I. The 2-guanidinoaminopyrimidine II (R = Me) formed as an intermediate in this reaction may be isolated, while II (R = Et) cyclizes to 2-amino-5-ethyl-7-trifluoromethyl-s-triazolo[1,5-a]pyrimidine.

RX(1) OF 4 A + B ===> C

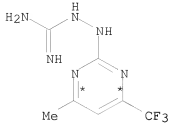


A



B

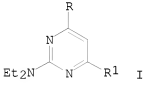
(1)



C
YIELD 16%

RX(1) RCT A 6882-47-9, B 367-57-7
PRO C 71999-95-6

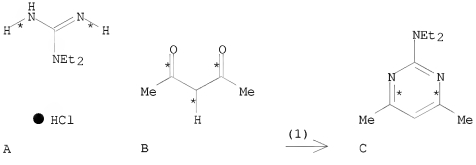
L3 ANSWER 96 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 90:54903 CASREACT
TITLE: 2-(Diethylamino)pyrimidines. Part 4. Analgesics
AUTHOR(S): Kreutzberger, A.; Leyke-Roehling, S.
CORPORATE SOURCE: Inst. Pharm., Freie Univ. Berlin, Berlin, Fed. Rep. Ger.
SOURCE: Arzneimittel-Forschung (1978), 28(11), 2051-4
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

AB Pyrimidines I (R = R1 = Me, Pr, CHMe2, Ph, 2-naphthyl; R = Me, R1 = Et, CH2CHMe2, Ph, 2-furyl, 2-thienyl) were prepared by condensing Et2NC(:NH)NH2 with RCOCH2COR1. I (R = R1 = Pr) has fungicidal activity against e.g. Septoria nodorum (no data).

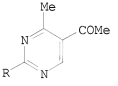
RX(1) OF 10 A + B ===> C



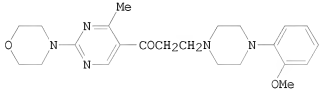
A B C

RX(1) RCT A 1114-39-2, B 123-54-6
PRO C 3036-77-9
CAT 497-19-8 Na2CO3

L3 ANSWER 97 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 88:170124 CASREACT
TITLE: Psychoactive agents. Part VI. Synthesis and central nervous system effects of some 2-substituted 5-acetyl-4-methylpyrimidine derivatives
AUTHOR(S): Arya, V. P.; David, J.; Grewal, R. S.; Marathe, S. B.; Patil, S. D.
CORPORATE SOURCE: Res. Cent., Ciba-Geigy, Bombay, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1977), 15B(12), 1129-32
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



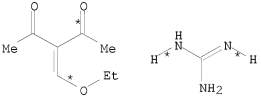
I



II

AB The synthesis of 2-substituted 5-acetyl-4-methylpyrimidines is described. Thus, amidines and substituted guanidines react with EtOCH:C(COMe)2 to give the 5-acetyl-4-methyl-2-substituted pyrimidines I (R = NH2, MeS, morpholino, Ph, etc.). Aminolysis of I (R = MeS) with cyclic secondary amines gave I (R = piperidino, piperazino, pyrrolidino, etc.). Some of these amines were converted to their guanylhydrazones. Mannich condensation of I (R = morpholino) gave II. Some I had central nervous system and bactericidal activity.

RX(2) OF 57 A + D ===> E...

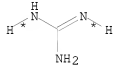


A D E
YIELD 94%

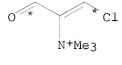
RX(2) RCT A 33884-41-2, D 113-00-8
PRO E 66373-25-9

L3 ANSWER 98 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 88:136580 CASREACT
TITLE: Synthetic reactions of dimethylformamide. Part XXXVII. Preparation, properties, and synthetic reactions of trimethylammoniodiformylmethylide
AUTHOR(S): Kral, V.; Arnold, Z.
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1977), 42(12), 3455-63
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The highly stabilized title ylide Me3N+C-(CHO)2 gave the 1:1 addition compds. with NaClO4, NaI, AgNO3, ZnI2, and HCl; 2-dimethylamino-3-methoxy-2-propenal by heating to .apprx.300°; and reactive salts (e.g. [ClCH:C(CHO)NMe3]+Cl- (I) with COCl2), which were used to prepare 5-, 6-, and 7-membered heterocycles with Me3N+ groups. Thus, I gave with hydrazine hydrate 88% of 4-trimethylammoniopyrazolium dichloride.

RX(6) OF 11 ...K + H ===> L

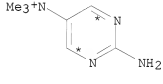


● HCl



● Cl⁻

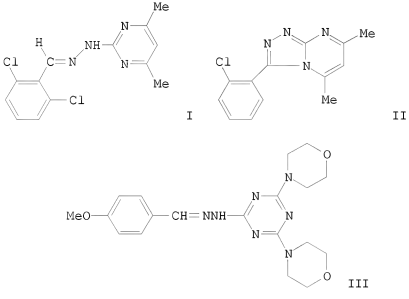
K H (6) L: CM 1
YIELD 86%



L: CM 2
YIELD 86%

RX(6) RCT K 50-01-1, H 65970-85-6
PRO L 65970-93-6

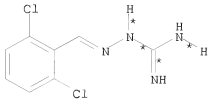
L3 ANSWER 99 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 88:135885 CASREACT
TITLE: Studies on heterocyclic compounds. V. Photochemical reactions of 2-(2,6-dichlorobenzylidenehydrazino)pyrimidine and its related hydrazones
AUTHOR(S): Tsujikawa, Teruaki; Tatsuta, Motomi
CORPORATE SOURCE: Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1977), 25(12), 3137-46
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



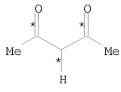
I II III

AB Under N, anti isomers, e.g., I, of 2-benzylidenehydrazinopyrimidines isomerized easily to their syn isomers under UV irradiation in C6H6. In the presence of O, photosensitized autoxidn. occurred to afford 3-aryl-1,2,4-triazolo-[4,3-a]pyrimidines, e.g., II. When irriated in the same manner, 2-benzylidenehydrazino-1,3,5-triazine derivs., e.g., III, decomposed to benzaldehydes, e.g., p-MeOC6H4CHO, and 2-hydroxy-1,3,5-triazines.

RX(5) OF 36 I + J ===> D...

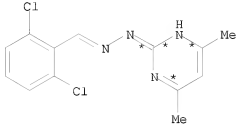


I



J

(5)

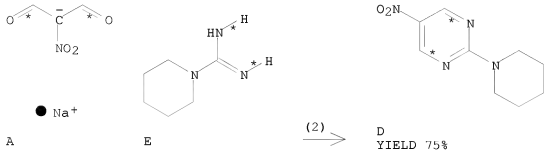


D
YIELD 30%

RX(5) RCT I 5051-62-7, J 123-54-6
PRO D 66957-88-8

L3 ANSWER 100 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 87:135248 CASREACT
TITLE: Reaction of sodium nitromalonic aldehyde with isothiuronium salts
AUTHOR(S): Maksimov, Yu. V.; Aleinikov, V. N.
CORPORATE SOURCE: USSR
SOURCE: Nekotor. Vopr. Khimii Redkozemel'n. Elementov (1975) 75-86
From: Ref. Zh., Khim. 1977, Abstr. No. 11Zh320
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.

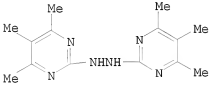
RX(2) OF 15 A + E ===> D

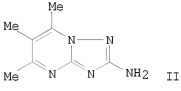


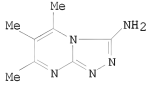
A E D
YIELD 75%

RX(2) RCT A 34461-00-2, E 4705-39-9
PRO D 64269-43-8

L3 ANSWER 101 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 85:21272 CASREACT
TITLE: Condensations with hydrazine-N,N'-dicarboxamidine, 20. Trisubstituted s-triazolo[1,5-a]pyrimidines
AUTHOR(S): Kreutzberger, Alfred; Kreutzberger, Elfriede
CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ. Muenster, Muenster, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1976), 309(2), 148-52
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

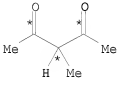

I

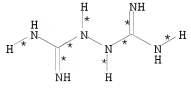

II


III

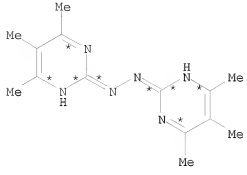
AB Condensation of [H2NC(:NH)NH]2 with MeCOCMe:C(OH)Me at room temperature gave only hydrazodipyrimidine I in 26.5% yield, but at 100°/6 hr, 52% yield of triazolopyrimidine II was primarily obtained, besides a little I. Triazolopyrimidine III was formed as an intermediate which rearranged to II via ring-opening of the pyrimidine portion. II was unambiguously synthesized from MeCOCMe:C(OH)Me and 3,5-diamino-s-triazole.

RX(1) OF 1 2 A + B ===> C


2 A


B

(1)

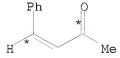


C
YIELD 26%

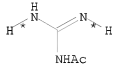
RX(1) RCT A 815-57-6, B 6882-47-9
PRO C 59444-01-8

L3 ANSWER 102 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 84:90106 CASREACT
TITLE: Pyrimidines. XLVII. New synthesis of 2-aminopyrimidines
AUTHOR(S): Mamaev, V. P.; Vais, A. L.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1975), (11), 1555-9
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The title compds. I [R = H, Ac; R1 = Ph, 4-(Me2N)C6H4, 4-O2NC6H4, Me, H; R2 = H, Ph, Me] were prepared by cycloaddn. of RNHC(NH2):NH with R1CH:CHCOR2.

RX(1) OF 16 A + B ===> C

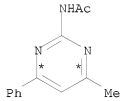


A



B

(1)

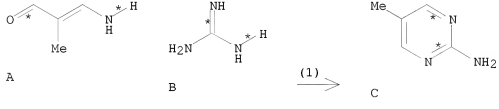


C
YIELD 41%

RX(1) RCT A 122-57-6, B 5699-40-1
RGT D 7782-44-7 O2
PRO C 15755-13-2

L3 ANSWER 103 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 82:140482 CASREACT
TITLE: Four routes for the synthesis of (2-pyrimidinylamino)-n-alkanoic acids
AUTHOR(S): Tjoeng, Foe-Siong; Kraas, Ekkehard; Stark, Erwin; Breitmaier, Eberhard; Jung, Guenther
CORPORATE SOURCE: Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1975), 108(3), 862-74
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Cycloaddn. of HCOCR:CHNH2 (R = Me, Pr, Bu, pentyl) with L-arginine gave N-(5-alkyl-2-pyrimidinyl)ornithines. Cycloaddn. of (MeCO)2CH2 with HZNC(:NH)R1 [I; R1 = NHCH2CO2H, NH(CH2)nCH(NH2)CO2H, n = 3,4, NMeCH2CO2H] gave the corresponding pyrimidines (II) in 46-64% yields. Pyrimidinylaminoalkanoic acids (III) were prepared by cycloaddn. of MeC(OH):CHCO2Et with I. Nucleophilic substitution of 2-ethylthio-4- or -5-methyl-6-oxo-1,6-dihydropyrimidine with R2H [R2 = NHCHR3CO2H, R3 = H, Me; R2 = NH(CH2)5CO2H, NH(CH2)4CH(NH2)CO2H] gave the corresponding III (R1 = R2) or IV, resp.

RX(1) OF 12 A + B ===> C



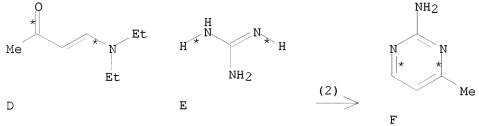
RX(1) RCT A 30989-81-2, B 113-00-8
PRO C 50840-23-8
CAT 124-41-4 NaOMe

L3 ANSWER 104 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 55:2707 CASREACT
TITLE: Derivatives of β-dicarbonyl compounds. II. Synthesis of 2,4-substituted pyrimidines
AUTHOR(S): Klimko, V. T.; Mikhalev, V. A.; Skoldinov, A. P.
SOURCE: Zhurnal Obshchei Khimii (1960), 30, 1258-64
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 51, 15449g. Adding 6 g. guanidine sulfate with cooling to 30 ml. concentrated H2SO4, then 8 g. AmCOCH:CHCl at 15-20°, heating the mixture over 2 hrs. to 90-5°, and quenching on ice gave 60.6% 2-amino-4-amylpyrimidine, m. 89-90°. Adding 13.4 g. guanidine nitrate to 8.4 g. NaOH in 50 ml. MeOH, then over 1.5 hrs. 10.4 g. MeCOCH:CHCl at 10-15°, and heating 5 hrs. on a steam bath gave after concentrating and extracting with CHCl3, 55% 2-amino-4-methylpyrimidine, m. 158-9°. Keeping 17 g. iso-BuCOCH:CHCl with 7.2 g. KOH in 90 ml. absolute EtOH 24 hrs. gave 62.1% iso-BuCH(OEt)2, b7 92°, n20D 1.4520, d20 0.9204, which (10.1 g.) heated with 4.5 g. guanidine carbonate 4 hrs. on a steam bath gave 66.2% 2-amino-4-isobutylpyrimidine, m. 118-19°. Heating 2.6 g. N-(β-benzoylvinyl)pyridinium chloride with 0.9 g. guanidine carbonate in MeOH 6 hrs., treating the product with 10% HCl, extracting the by-product AcPh with Et2O, addg. alkali to the aqueous layer, and extracting with CHCl3 gave 23.3% 2-amino-4-phenylpyrimidine, m. 160-1°. Adding 12 g. o-BrC6H4COCH:CHCl in 25 ml. EtOH to 3 g. KOH in dry EtOH with cooling gave after 12 hrs. at room temperature 80.6% o-BrC6H4COCH:CHOEt, b3 150-3°, d20 1.4110, n20D 1.5612, which heated 4 hrs. with guanidine carbonate in MeOH gave 89.2% 2-amino-4-(o-bromophenyl)pyrimidine, m. 163-4°. To 0.46 g. Na in dry EtOH was added 1.9 g. guanidine HCl salt followed by 2.8 g. MeCOCH:CHNEt2, and the whole heated 16 hrs. on a steam bath to give 82.5% 2-amino-4-methylpyrimidine, m. 157.5-8.5°. To 7 g. NaOH in 50 ml. MeOH was added at 0° 9 g. benzamidine HCl salt, followed by 6 g. MeCOCH:CHCl and the mixture refluxed 5 hrs. to give 62% 2-phenyl-4-methylpyrimidine, m. 25°, b. 275-9°. To 25 ml. 96% H2SO4 was added 8 g. N-phenylguanidine carbonate at 0°, then at 15-20° 5.2 g. MeCOCH:CHCl, the mixture kept 2 hrs. at 90-5°, and quenched in ice to yield 54% 2-phenylamino-4-methylpyrimidine, m. 92-3°. Heating 2.02 g. iso-BuCOCH2CH(OEt)2 with 1.66 g. N-phenylguanidine carbonate 4 hrs. at 160° gave after quenching in ice and treatment with 1:4 HNO3 at pH 3, 74.8% 2-phenylamino-4-isobutylpyrimidine, m. 49-50°. To 120 g. NaOH in 1.5 l. MeOH was added 214 g. sulfanilylguanidine, then at 50-60° 104.5 g. MeCOCH:CHCl, the mixture refluxed 5 hrs., filtered, and the precipitate taken up in H2O, treated with C and acidified to pH 7 with HCl to yield 50% 2-sulfanilamido-4-methylpyrimidine, m. 231-2°. Similar procedures also gave [% yield and m.p. (b.p./mm.) shown]: 64.5, 2-amino-4-ethylpyrimidine, 136°; 86.9, 2-amino-4-propylpyrimidine, 122-3°; 63, 2-amino-4-p-nitrophenylpyrimidine, 170-1°; 59.7, 2-amino-4-p-anisylpyrimidine, 189-90°; 35.2, 2-phenyl-4-ethylpyrimidine, (135-40°/5, d20 1.0803, n20D 1.5840); 40.6, 2-phenyl-4-propylpyrimidine, (153-5°/10 1.0501, 1.5795); 53.6, 2,4-diphenylpyrimidine, 71-2°, (197-8°/5); 42.2, 2-phenylamino-4-ethylpyrimidine, 55-6°; 53.7, 2-phenylamino-4-propylpyrimidine, 54-5° (b7 177°); 70.2,

2-phenylamino-4-amylpyrimidine, isolated as the nitrate; 72.8,
2-phenylamino-4-phenylpyrimidine, 137-8°; 37,
2-sulfanilamido-2-ethylpyrimidine, 240-1°; 51.5,
2-sulfanilamido-4-propylpyrimidine, 216-17°; 32.2,
2-sulfanilamido-4-isobutylpyrimidine, 227-8°; 29.4,
2-sulfanilamido-4-amylpyrimidine, 225-6°; 23,
2-sulfanilamido-4-phenylpyrimidine, 261-2°.

RX(2) OF 2 D + E ===> F



D E F
YIELD 83%

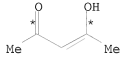
RX(2) RCT D 38664-61-8, E 113-00-8
PRO F 108-52-1
SOL 64-17-5 EtOH
NTE Classification: Heterocycle formation; Condensation; # Conditions: EtOH; 1h36mn water bath; # Comments: H2NC(=NH)NH2 used as HCl salt; Free guanidine formed from its hydrochloride using Na EtOH

L3 ANSWER 105 OF 105 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 54:34303 CASREACT
TITLE: Condensations with 1,2-hydrazinedicarboxamidine. 2,2'-Hydrazopyrimidines
AUTHOR(S): Kreutzberger, Alfred
CORPORATE SOURCE: Ford Motor Co., Dearborn, MI
SOURCE: Journal of the American Chemical Society (1959), 81, 6017-21
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

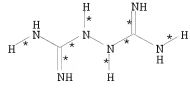
AB The condensation of 1,2-hydrazinedicarboxamidine (I) with β-diketones to the corresponding 2,2'-hydrazopyrimidines was investigated. Aminoguanidine bicarbonate (300 g.) added in portions to 1400 cc. 70% HNO3, diluted with 1000 g. crushed ice, treated at 0-10° with saturated aqueous KMnO4 in portions, kept overnight at 0°, and filtered gave 70-80 g. azodicarboxamidine dinitrate (II). The II in 350-400 cc. H2O treated with occasional shaking with a stream of H2S, filtered, kept overnight, refiltered, and evaporated in vacuo yielded 65-75 g. I.2HNO3.H2O, m. 137-9° (decomposition). MeCOEt (72 g.) added at 0° with stirring to 23 g. Na powder in 352 cc. EtOAc, kept overnight, heated 1.5 hr. on the steam bath, kept 3 days at room temperature, acidified with glacial AcOH to pH 6, poured onto 500 g. crushed ice, the aqueous layer extracted with Et2O, and the combined organic layer and extract worked up gave 57.6 g. AcCH2COEt, b12 54-5°. Similarly was prepared (EtCO)2CH2, n18D 1.4470, in 48.6% yield. Ac2CH2 (20 g.) and 92 g. 30% aqueous K2CO3 added to 26.0 g. I.2HNO3.H2O in 90 cc. lukewarm H2O and filtered after 1 week yielded 16.8 g. 4,4',6,6'-tetramethyl-2,2'-hydrazopyrimidine (III), prisms, m. 224-5° (EtOH); N,N'-di-Ac derivative m. 167°. Similarly were prepared the following compds. (% yield, m.p., and m.p. of N,N-di-Ac derivative given): tetra-Et analog of III, 94, 128-9°, 111-12°; 4,4'-dimethyl-6,6'-diethyl analog of III, 71.4, 129-30°, 137-8°; 4,4',5,5',6,6'-hexa-Me analog of III, 68.5, 264-5°, 209-10°. III (0.7 g.) in 10 cc. Ac2O heated 1.5 hrs. on the steam bath, cooled, evaporated, the residue dissolved in 2 cc. glacial AcOH, the solution treated with C, diluted with 15 cc. H2O, and the product filtered off yielded the N,N'-di-Ac derivative of III, m. 167°. (EtO2C)2CHCH:C(CO2Et)2 Na derivative (35.2 g.) in 600 cc. H2O added gradually at room temperature to 13 g. I.2HNO3.H2O in 50 cc. H2O, filtered after 2.5 hrs., allowed to stand, and the precipitate recrystd. from hot HCONMe2 yielded 3.1 g. 4,4'-dihydroxy-5,5'-dicarbethoxy-2,2'-hydrazopyrimidine (IV), m. 227-8°. I.2HNO3.H2O (6.5 g.) in 20 cc. lukewarm H2O treated with 20 g. 10% aqueous NaOH and 10.8 g. EtOCH: C(CO2Et)2 and filtered after a few days, and the residue extracted with hot H2O gave 1.9 g. IV, m. 227-8°; the aqueous extract cooled deposited 2.4 g. 5,5'-di-CO2H analog of IV, m. 216-17°. I.2HNO3.H2O (13 g.) treated with 40 g. aq 10% NaOH, the mixture then treated with 13 g. AcCH2CO2Et and kept 3 weeks, and the crystalline deposit triturated with Et2O yielded 3.3 g. 1,2-bis(acetoacetylguanyl)hydrazine, m. 228-30°. I.2HNO3.H2O (13 g.) in 40 cc. H2O treated with 40 g. 10% aqueous NaOH and 22.6 g. NCCH2CO2Et, kept 4 weeks, and filtered yielded 9.6 g. dicyanoacetate (V) of I, needles, m. 203-4° (effervescence) (H2O). NCCH2CO2H (3.4 g.) in 5 cc. H2O, and 16 g. 10% aqueous NaOH added to 5.2 g. I.2HNO3.H2O in 17 cc. warm H2O, kept 2 days, and filtered gave 4.1 g. V, m. 203-4° (effervescence). CH2(CO2Et)2 (9.6 g.) and 33 g. 10% aqueous KOH added to 7.8

g. I.2HNO3.H2O in 20 cc. H2O, kept 2 weeks, and filtered yielded 3.9 g. (crude) malonate (VI) of I, prisms, m. 216-17° (bubbling) (H2O). CH2(CO2H)2 (2.1 g.) in 3 cc. H2O and 22 g. 10% aqueous KOH added to 5.2 g. I.2HNO3.H2O in 15 cc. warm H2O and filtered after 3 days yielded 2.8 g. VI.

RX(2) OF 2 2 E + F ===> G

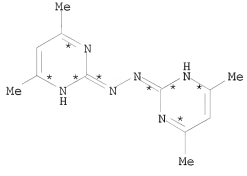


2 E



F

(2)



G
YIELD 70%

RX(2) RCT E 26567-75-9, F 6882-47-9
RGT H 584-08-7 K2CO3
PRO G 7135-09-3
SOL 7732-18-5 Water
NTE Classification: Heterocycle formation; Condensation; # Conditions: K2CO3 H2O; 1 week; # Comments: di-guanidine as dinitrate salt and monohydrate

```
=> d his

     (FILE 'HOME' ENTERED AT 18:20:08 ON 07 NOV 2008)

     FILE 'CASREACT' ENTERED AT 18:20:44 ON 07 NOV 2008
L1             STRUCTURE UPLOADED
L2          152 S L1 FULL
L3          105 S L2 AND PY<2003

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    654.03     654.24

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -78.75     -78.75

STN INTERNATIONAL LOGOFF AT 18:24:53 ON 07 NOV 2008
```